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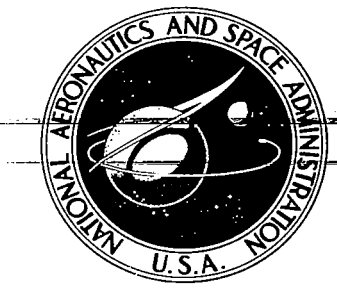

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COMBUSTION OF HYDROGEN INJECTED INTO A SUPERSONIC AIRSTREAM (THE SHIP COMPUTER PROGRAM)

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16. Abstract

This report details the mathematical and physical basis of the SHIP computer program which embodies a finite-difference, implicit numerical procedure for the computation of hydrogen injected into a supersonic airstream at an angle ranging from normal to parallel to the airstream main flow direction. The physical hypotheses built into the program include: a two-equation turbulence model, and a chemical-equilibrium model for the hydrogen-oxygen reaction.

Typical results for equilibrium combustion are presented and exhibit qualitatively plausible behavior. The computer time required for a given case is approximately 1 minute on a CDC 7600 machine.

A discussion of the assumption of parabolic flow in the injection region is given which suggests that improvement in calculation in this region could be obtained by use of the partially-parabolic procedure of Pratap and Spalding.

It is concluded that the technique described herein provides the basis for an efficient and reliable means for predicting the effects of hydrogen injection into supersonic airstreams and of its subsequent combustion.

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NOMENCLATURE

A_i, A'_i	Coefficients in the finite-difference equations.
B	Source term in the finite-difference expression inclusive of upstream convection.
C_1, C_2, C_D	Constants in the turbulence model.
c_p	Specific heat at constant pressure.
D	Coefficient relating pressure gradients to velocities.
E	East, grid node East of P, constant in the log law.
e	Location on grid.
f	Mass fraction of hydrogen in any form.
G	Generation of kinetic-energy of turbulence.
$\bar{h}$	Stagnation enthalpy.
h^o_i	Enthalpy of formation.
K	Constant in law-of-wall.
k	Kinetic-energy of turbulence.
L^i	The convection coefficient in the finite-difference equations.
ℓ	Turbulence length scale.
m	Entrained mass from the free boundary.
$\bar{m}$	The total inflow from the inlet boundary.
$\dot{m}$	Local mass-imbalance at any finite-difference cell - defined as (outflow-inflow).
mf_i	Mass fraction of species i.

N	North, grid node North of P.
n	Location on grid.
P	Refers to grid node of interest.
p	Pressure used in lateral-momentum equation.
p'	Pressure correction.
$\bar{p}$	Pressure used in the longitudinal momentum equation.
Pr	Prandtl number.
P_ϕ	Resistance of laminar sublayer used in the wall-functions.
R	Gas constant used to define the density.
S	South, grid node South of P.
S^ϕ	Integrated source term of ϕ over the volume. $S^\phi = s^\phi$ x volume of the control volume.
s^ϕ	Source term of ϕ per unit volume.
T	Temperature
T^i_j	The diffusive coefficient in the finite-difference equations.
u v w	The velocity components along ξ, η and ζ directions respectively, location on grid.
u' v' w'	Velocity corrections
u^* v^* w^*	The uncorrected velocity components along ξ, η and ζ directions, respectively,
W	West, grid node West of P, molecular weight.
y_p	Distance of near wall grid node from a wall.

x, y, z	Cartesian coordinates.

Greek Symbols

Γ_ϕ	Exchange coefficient in ϕ equation.
γ	Ratio of specific heats, c_p/c_v.
ϵ	Dissipation rate of kinetic energy of turbulence.
ξ,η,ζ	Quasi-orthogonal coordinate system.
μ	Viscosity.
μ_t	Turbulent viscosity.
ρ	Density of the fluid.
σ_ϕ	Laminar Prandtl or Schmidt number for ϕ.
$\sigma_{t,\phi}$	Turbulent Prandtl or Schmidt number for ϕ.
τ	Shear stress.
ϕ	General flow property.

Subscripts

D	Pertaining to downstream.
e,w,n,s	Locations on grid.
E,W,N,S	Value of variable at the East, West, North, South location, respectively.
i,j	X- and Y- direction location on grid.
P	Denotes value at point P.
U	Value of variable at the upstream location.
ϕ	Property for a general variable ϕ.
ref	Reference value.

Superscripts

u,v,w	Pertain to the three velocity-components.
p'	Values for the pressure-correction equation.
ξ,η,ζ	Denote the quantities along the respective coordinate-directions.
ϕ	Value in the equation for a ϕ variable

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1. INTRODUCTION

1.1 Background

The SHIP (Supersonic Hydrogen Injection Program) computer program is concerned with the numerical computation of three-dimensional flow situations arising when hydrogen is injected into a supersonic airstream at an angle ranging from normal to parallel to the airstream main flow direction. The flow may be free, or confined in a duct whose walls may expand or contract arbitrarily but smoothly.

In its present version, SHIP predicts the mass fractions of the products of combustion of hydrogen and oxygen based on the assumption of chemical equilibrium.

1.2 Connections with Previous Work

Under a previous Contract (NAS1-13239) a computer program, HISS, was developed for similar situations to those considered here. The code has been extended and extensively modified to become SHIP so that the following facilities, not provided for in HISS, are included:

(i) Any of the four lateral boundaries can be (1) a wall, (2) a symmetry plane, (3) a free surface.

(ii) For walls, the distance of each wall from a reference plane may be specified as an arbitrary, but smooth, function of distance along the principal flow direction.

(iii) Ability to specify mass flux through the top and bottom wall is provided.

(iv) Choice between specification of an adiabatic wall or a constant temperature on each wall is provided.

1.3 Purpose of the Present Report

The terms of the NASA contract call for the development and transmission of the SHIP code having the general features described above.

This report marks the completion of the project. It provides all the necessary information concerning the mathematical modelling of the flows under consideration, it describes the numerical analysis involved in the solution of the relevant equations and it defines the user-orientated parts of the code.

It is to serve as both a comprehensive reference to the mathematics and numerical procedure used in the code and as an operational manual for the computer program SHIP.

1.4 The Physical Problem Considered

NASA is active in research on supersonic combustion {2-4}. Of particular interest are methods for injecting hydrogen in a supersonic airstream in a manner which optimizes the design of supersonic combustors.

Three arrangements of interest are shown in Figures (1), (2) and (3).

Due to interaction of the mainstream with the jet, the flow separates ahead of the jet and reattaches behind it. Also a bow shock is caused by this interaction.

There is an interaction between the jets causing flow in directions normal to the main-stream direction. This is the phenomenon which makes three-dimensional calculations necessary.

Downstream of the jet the hydrogen mixes with the air and the region containing hydrogen widens.

As the flow moves downstream, the mixing, chemical reaction, acceleration, viscous effects etc. all combine to produce a pressure variation.

Thus, in addition to the aero- and thermodynamic characteristics of these flow arrangements, knowledge of the extent of the region of hydrogen, and its distribution within it, is necessary to assess the effectiveness and uniformity of air-hydrogen mixing.

1.5 Capabilities and Limitations of SHIP

SHIP is a general, flexible computer program capable of calculating three-dimensional, boundary-layer flows which are either external or internal. Features built into this program include:

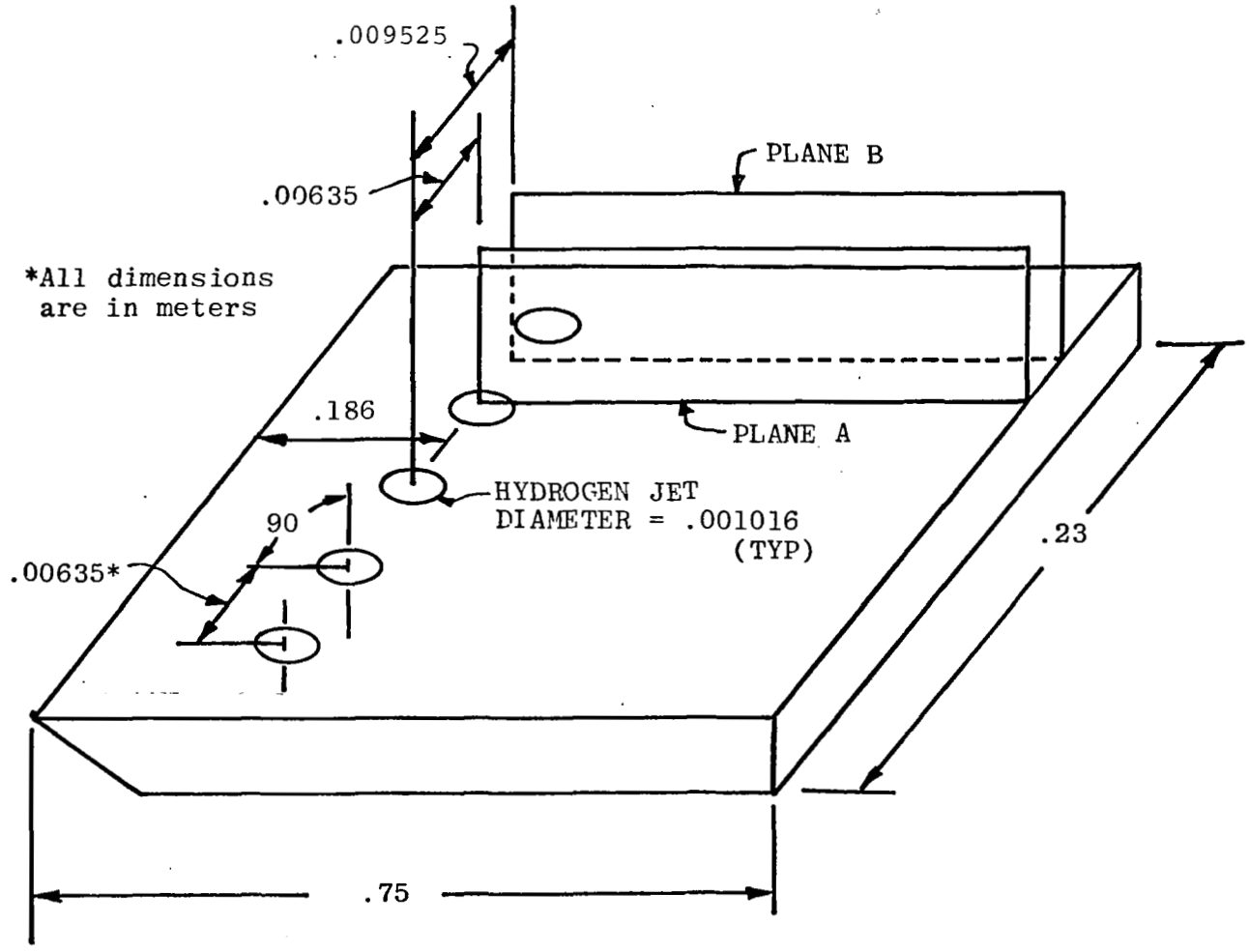


FIGURE 1: DEFINITION OF GEOMETRY AND PLANES OF PROFILES FOR CASE 1

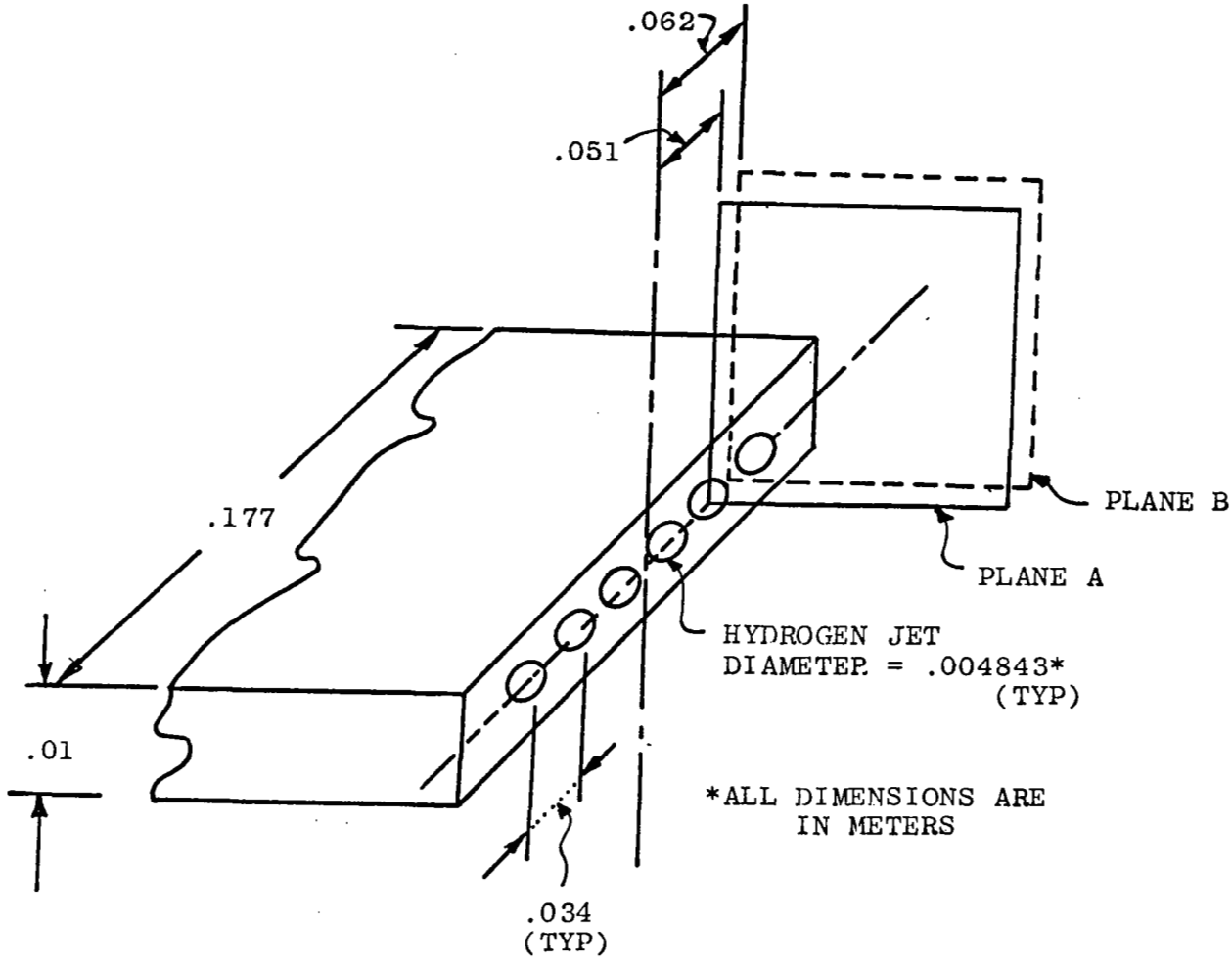
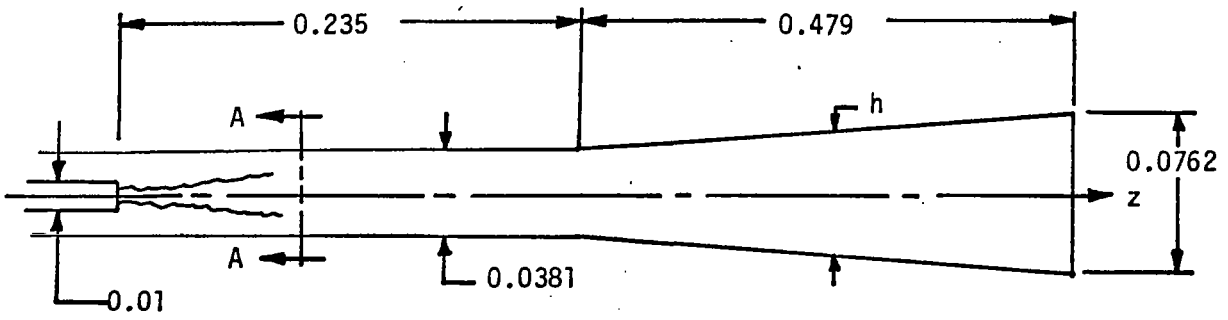
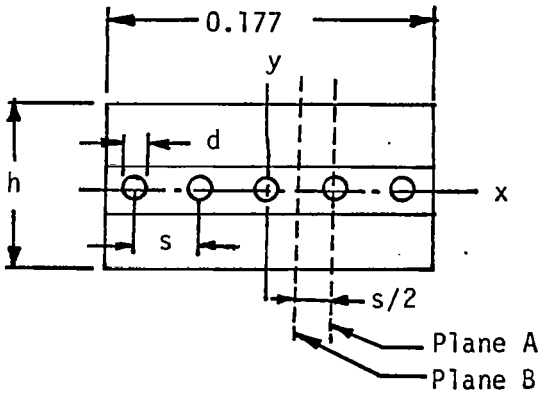


FIGURE 2: DEFINITION OF GEOMETRY AND PLANES OF PROFILES FOR CASE 9

NOTE: All dimensions in meters





SECTION A-A

NOTE: Calculations are performed between boundaries shown in the view at the right.

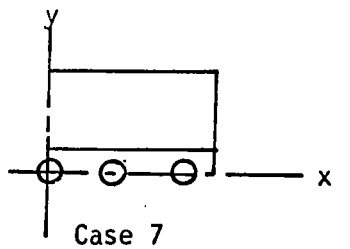


FIGURE 3: DEFINITION OF CASE 7 TO DEMONSTRATE THE VALIDITY OF THE SHIP CODE

- Any of the four boundaries can be either a wall, a symmetry plane, or a free surface.
- For internal flows the distance of the duct walls from a reference plane may be specified as a function of distance along the principal flow direction.
- Walls can be specified as being either adiabatic or at constant temperature.
- Injection of hydrogen at angles ranging from normal to parallel to the main air-stream can be handled.
- Injection through arrays of holes in either or both the top and bottom walls is provided for.
- Free-boundary conditions resulting from a small-disturbance theory and isentropic considerations are applied to supersonic free boundaries.

Thermodynamic equilibrium is supposed to prevail between the species H_2, O_2, H_2O, O, H and OH; and four equilibrium reactions are allowed for.

The upper surface of the domain of integration is taken above the bow shock so that the edge conditions may be the same as the free-stream conditions.

The lateral and longitudinal pressure gradients are uncoupled in the subsonic-flow in order that the equations remain parabolic, and forward-marching integration can be used; thus, the calculation "jumps" the separated region at the jet exit.

The practice used for this jump is as follows:

1. An arbitrary long forward step is taken over the jet exit [e.g., 10 jet diameters]. This effectively jumps the elliptic region near the jet exit.

2. The source and sink terms for all of the dependent variables are modified at the cell immediately over the jet exit, so as to account for the required inflow rate at the jet boundary of the variable in question. The overall conservation of mass, momentum, and energy, is thus satisfied for the region over the jet.

The flow is considered to be turbulent and the effective viscosity is calculated by way of the "k-ε" two equation turbulence model described in {5}. Density is calculated via the ideal-gas law.

The program predicts the distributions of the following variables:

(i) the three velocity components;
(ii) static pressure;
(iii) total enthalpy;
(iv) mass fraction of each species present in the field, i.e. H_2, H, O_2, O, H_2O, OH, N_2.

(v) turbulence energy and dissipation rate of turbulence energy.

The program also predicts the distributions of auxiliary quantities; namely, temperature and density distributions, and drag and heat transfer at the walls.

The program is written in standard FORTRAN IV language and, although it has been developed on a CDC machine, it will require only minor modifications to run on other machines with FORTRAN IV compilers.

1.6 Outline of this Report

The remainder of this report is divided into the following eleven Chapters:

Chapter 2 is concerned with the mathematical formulation and physical models employed in SHIP.

Chapter 3 then describes the finite-difference equations and outlines the numerical solution algorithm for solving the relevant equations.

Chapters 4 to 8 are devoted to program topics and are intended primarily as the operational manual for the program.

Emphasis is therefore placed on the description of the program structure, the function of the subroutines and on the input/output features. These sections provide all necessary instructions to permit formulation of problems which fall within the scope of SHIP. It also provides information to aid interpretation of the predictions obtained from the program.

In Chapter 9, sample predictions for some test cases specified by NASA Langley are discussed. Suggestions for further extensions and refinements of SHIP are included in Chapter 10.

Relevant literature references (Chapter 11) and nomenclature (Chapter 12) close this report.

Appendix A describes in detail the equilibrium chemistry model used in conjunction with the computer program to predict the properties in a hydrogen-oxygen flame.

Appendix B describes the Free Stream Boundary Conditions in supersonic flows.

Finally, Appendix C gives a list of FORTRAN variables used in SHIP and a listing of the SHIP program is provided in Appendix D.

The present report supersedes a previous CHAM report published as NASA CR-2655, March 1976 {6}.

2. THE MATHEMATICAL AND PHYSICAL ANALYSIS

2.1 Introduction

This chapter details the mathematical and physical basis of the SHIP code. Section 2.2 is concerned with the system of coordinates chosen for use in the present work. Section 2.3 is concerned with giving the differential equations for conservation of momentum, stagnation enthalpy and chemical species.
Section 2.4 describes the turbulence model. Finally, Section 2.5 provides the auxiliary information necessary to close the problem.

2.2 The Coordinate System

The system of coordinates chosen for use in the present work, is quasi-orthogonal. The reason for this choice is that the representation of flows within domains whose cross-sections vary with axial position cannot conveniently be achieved through equations expressed in orthogonal coordinate systems. It is stipulated that whereas two of the coordinate axes (x,y) maintain mutual orthogonality throughout the flow-field, the third (z) is permitted to depart from orthogonality with respect to the other two, within specified limits. It is demonstrated below that these limits are consistent with the boundary-layer approximations {7}.

The elements of the curvilinear system (ξ,η,ζ) are defined in terms of orthogonal, Cartesian coordinates (x,y,z) as follows:

$$\xi = \frac{x - x_W}{x_E - x_W} \quad (a)$$

$$\eta = \frac{y - y_S}{y_N - y_S} \quad (b) \qquad (2.2\text{-}1)$$

and $$\zeta = z \quad (c)$$

Furthermore we define:

$$\Delta\xi_W = x_w \quad (a)$$

$$\Delta\xi_E = x_e - x_w \quad (b)$$

$$\Delta\eta_S = y_s \quad (c) \qquad (2.2\text{-}2)$$

$$\Delta\eta_N = y_n - y_s \quad (d)$$

The above definitions can best be appreciated with reference to Figure (4). The subscripts N, S, E and W, refer respectively to the North, South, East and West boundaries of the calculation domain in the x-y plane.

The coordinates η and ξ are mutually orthogonal for all values of ζ. Furthermore, planes of constant ζ are approximated as planes of constant z.

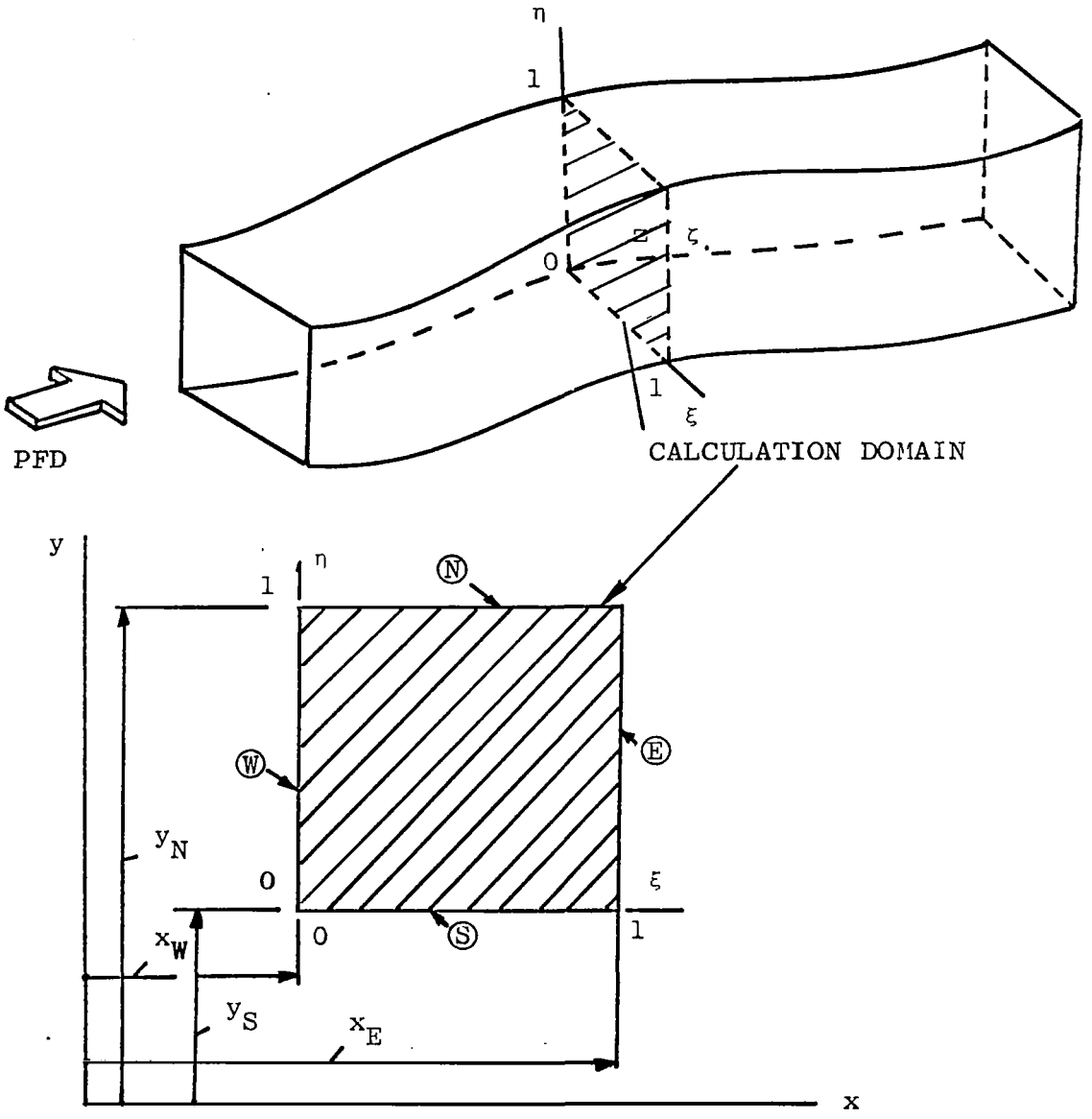


FIGURE 4: ILLUSTRATION OF THE QUASI-ORTHOGONAL COORDINATE SYSTEM; THE CIRCLED CHARACTERS REPRESENT THE NORTH, SOUTH, EAST AND WEST BOUNDARIES OF THE CALCULATION DOMAIN

The above definitions for η,ξ make possible the use of coordinates that vary between 0 and 1 only.

The components of velocity u, v and w are now defined as follows: u and v are normal to the y-z and z-x planes respectively, i.e. are aligned with the ξ and η coordinate directions. w is normal to constant ζ planes, but is permitted to depart from alignment with ζ by small angles; the limits of this inclination are prescribed below. The following mathematical consequences result from the above definitions.

The coordinates (ξ,η,ζ) satisfy the general relationships:

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial x} + \frac{\partial}{\partial \zeta}\frac{\partial \zeta}{\partial x}$$

$$\frac{\partial}{\partial y} = \frac{\partial}{\partial \xi}\frac{\partial \xi}{\partial y} + \frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial y} + \frac{\partial}{\partial \zeta}\frac{\partial \zeta}{\partial y} \qquad (2.2\text{-}3)$$

$$\frac{\partial}{\partial z} = \frac{\partial}{\partial \xi}\frac{\partial \xi}{\partial z} + \frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial z} + \frac{\partial}{\partial \zeta}\frac{\partial \zeta}{\partial z}$$

which on application of the definitions of (2.2-1) and (2.2-2) reduce to:

$$\frac{\partial}{\partial x} = \frac{1}{\Delta \xi_E}\frac{\partial}{\partial \xi}$$

$$\frac{\partial}{\partial y} = \frac{1}{\Delta \eta_N}\frac{\partial}{\partial \eta} \qquad (2.2\text{-}4)$$

$$\frac{\partial}{\partial z} = -\frac{1}{\Delta \xi_E}\left\{\frac{\partial \Delta \xi_W}{\partial z} + \xi\frac{\partial \Delta \xi_E}{\partial z}\right\}\frac{\partial}{\partial \xi}$$

$$-\frac{1}{\Delta \eta_N}\left\{\frac{\partial \Delta \eta_S}{\partial z} + \eta\frac{\partial \Delta \eta_N}{\partial z}\right\}\frac{\partial}{\partial \eta} + \frac{\partial}{\partial \zeta}$$

It can be deduced that, on applying the definitions (2.2-1) to relationships (2.2-3), the effect of non-orthogonality of

the ζ coordinate with respect to ξ and η is negligible only if the following conditions are satisfied:

$$\frac{\partial \zeta}{\partial z} \approx 1 \qquad \text{(a)}$$

$$\frac{\partial \eta}{\partial z} \; ; \; \frac{\partial \xi}{\partial z} << 1 \qquad \text{(b)} \qquad \text{(2.2-5)}$$

Conditions (b) are similar to the well-known boundary-layer assumptions; thus the definitions (2.2-1) along with conditions (2.2-5) permit the transport equations to be expressed in quasi-orthogonal coordinates, whilst retaining their boundary-layer character.

The conditions (2.2-5(b)) are related to the area-ratio variation along the axis. It is obvious that this variation must be small to maintain the desired unstalled flow regime. Since stall, or axial flow recirculation, violates the conditions required for boundary-layer flows (i.e. flows within the range of validity of SHIP), the above conditions are consistent with the physical nature of the flows under consideration.

2.3 The mean-flow Conservation Equations

The differential equations listed in this section are the ones which express the conservation of momentum, mass, energy and chemical species in a three-dimensional flow with axial variations in cross-section.

The form of these equations is restricted to flows which are classified as parabolic/hyperbolic. The term "parabolic flows" implies that:

(a) there exists a predominant direction of flow (i.e. there is no reverse flow in that direction);

(b) the diffusion of momentum, heat, mass etc. is negligible in that direction, and

(c) the downstream pressure field has little influence on the upstream flow conditions.

When these conditions are satisfied, the coordinate in the main-flow direction becomes a "one-way" coordinate: i.e. the upstream conditions can determine the downstream flow properties, but not vice versa. It is this convenient

behaviour of the parabolic flows that allows the use of a marching integration from an upstream station to a downstream one, for the solution of the following equations.

a. Continuity

$$\frac{1}{\Delta\xi_E}\frac{\partial}{\partial\xi}\left\{(\rho u - \rho w\{\frac{d}{dz}(\Delta\xi_W) + \xi\frac{d}{dz}(\Delta\xi_E)\})\right\} +$$

$$\frac{1}{\Delta\eta_N}\frac{\partial}{\partial\eta}\left\{(\rho v - \rho w\{\frac{d}{dz}(\Delta\eta_S) + \eta\frac{d}{dz}(\Delta\eta_N)\})\right\} +$$

$$\frac{1}{\Delta\xi_E\Delta\eta_N}\frac{\partial}{\partial\zeta}(\Delta\xi_E\Delta\eta_N\,\rho w) = 0 \qquad (2.3\text{-}1)$$

b. Transport of fluid property ϕ

$$\frac{1}{\Delta\xi_E}\frac{\partial}{\partial\xi}\left\{(\rho u - \rho w\{\frac{d}{dz}(\Delta\xi_W) + \xi\frac{d}{dz}(\Delta\xi_E)\})\phi\right\} +$$

$$\frac{1}{\Delta\eta_N}\frac{\partial}{\partial\eta}\left\{(\rho v - \rho w\{\frac{d}{dz}(\Delta\eta_S) + \eta\frac{d}{dz}(\Delta\eta_N)\})\phi\right\} +$$

$$\frac{1}{\Delta\xi_E\Delta\eta_N}\frac{\partial}{\partial\zeta}(\Delta\xi_E\Delta\eta_N\,\rho w\phi) = S_\phi + \frac{1}{(\Delta\xi_E)^2}\frac{\partial}{\partial\xi}$$

$$\left\{\Gamma_\phi\frac{\partial\phi}{\partial\xi}\right\} + \frac{1}{(\Delta\eta_N)^2}\frac{\partial}{\partial\eta}\left\{\Gamma_\phi\frac{\partial\phi}{\partial\eta}\right\} \qquad (2.3\text{-}2)$$

In the above equation, ϕ is taken to represent any fluid property transported by the flow, including the three components of momenta per unit mass, u, v and w. The quantities within square brackets are consequences of the curvilinear nature of the geometry confining the flow. The terms S_ϕ and Γ_ϕ represent respectively the source (and/or sink) and the diffusion coefficient for the transport of ϕ.

The nature of the dependent variables and the associated forms of S_ϕ and Γ_ϕ are given in Table (1); and other symbols are defined in Section (12). The Table shows that the particular versions of (2.3-2) of interest here are: the momentum equations for each coordinate direction; the energy equation; an equation expressing conservation of total hydrogen; and the differential equations for turbulence properties. These equations together with the continuity equation (2.3-1) permit calculation of eight dependent variables, namely, $u,v,w,p,f,\bar{h},k$ and ε.

The omissions from the equations are the shear stresses and diffusion fluxes acting in the z-direction. These omissions accord with the definition of parabolic flows and with the consequent necessity to ensure that no influence from downstream can penetrate upstream.

A further point to note is that in subsonic flows the symbol $\bar{p}$ used for the pressure in the z-momentum equation is different from the symbol p in the two other momentum equations. This is a reminder of the fact that in the calculation procedure an inconsistency is deliberately introduced into the treatment of pressure, and that the quantities $\bar{p}$ and p are calculated differently. The pressure $\bar{p}$ can be thought of as a form of space-averaged pressure over a cross-section, and the gradient $\partial\bar{p}/\partial\zeta$ is supposed to be known (or calculated) before calculation of the lateral gradients $\partial p/\partial\eta$, $\partial p/\partial\xi$. This practice is implicit in two-dimensional boundary-layer theories also. It is the final step to be made in preventing downstream influences from propagating upstream. If this step is omitted the solution is often wholly unrealistic physically. This inconsistency in the treatment of pressure, it may be said, is one part of the price to pay for making the equations parabolic; the gain is the freedom to employ marching integration and to use two-dimensional computer storage, even though the flow is three-dimensional and the full equations are elliptic. There is however no penalty for wholly supersonic flows, for which the three momentum equations can share the same pressure, without impairing the marching-integration feature.

2.4 The Turbulence Model

The effective turbulent-transport coefficients μ_{eff}, Γ_k, Γ_ε, $\Gamma_{\bar{h}}$ and Γ_f are determined by means of a two-equation (k-ε) model of turbulence {5}. According to this model, the magnitude of the viscosity depends only on the local values of the turbulence kinetic energy, k, on the dissipation rate of turbulence energy, ε, and on the fluid density ρ.

The form of the two transport equations for k and ε is identical to (2.3-2); the transport coefficients and source terms are provided in Table (1)

TABLE (1)

The appropriate transport coefficients and source terms for the variable ϕ

ϕ	Γ_ϕ	S_ϕ
u	μ_{eff}	$\frac{1}{(\Delta\xi_E)^2}\frac{\partial}{\partial\xi}\left[\mu_{eff}\frac{\partial u}{\partial\xi}\right] - \frac{1}{\Delta\xi_E}\frac{\partial p}{\partial\xi} + \frac{1}{\Delta\xi_E\Delta\eta_N}\frac{\partial}{\partial\eta}\left[\mu_{eff}\frac{\partial v}{\partial\xi}\right]$
v	μ_{eff}	$\frac{1}{(\Delta\eta_N)^2}\frac{\partial}{\partial\eta}\left[\mu_{eff}\frac{\partial v}{\partial\eta}\right] - \frac{1}{\Delta\eta_N}\frac{\partial p}{\partial\eta} + \frac{1}{\Delta\xi_E\Delta\eta_N}\frac{\partial}{\partial\xi}\left[\mu_{eff}\frac{\partial v}{\partial\eta}\right]$
w	μ_{eff}	$-\frac{\partial\bar{p}}{\partial\zeta}$
k	$\frac{\mu_t}{\sigma_{t,k}}$	$\mu_t\Big\{2\{(\frac{1}{\Delta\xi_E})^2(\frac{\partial u}{\partial\xi})^2 + (\frac{1}{\Delta\eta_N})^2(\frac{\partial v}{\partial\eta})^2\} + \frac{1}{(\Delta\xi_E)^2}(\frac{\partial w}{\partial\xi})^2 + \frac{1}{(\Delta\eta_N)^2}(\frac{\partial w}{\partial\eta})^2 + \{\frac{1}{\Delta\xi_E}(\frac{\partial v}{\partial\xi}) + \frac{1}{\Delta\eta_N}(\frac{\partial u}{\partial\eta})\}^2\Big\} - \rho\varepsilon \equiv G_k - \rho\varepsilon$
ε	$\frac{\mu_t}{\sigma_{t,\varepsilon}}$	$\frac{\varepsilon}{k}(C_1 G_k - C_2 \rho\varepsilon)$
$\bar{h}$	$\frac{\mu_t}{\sigma_{t,\bar{h}}}$	$\frac{1}{(\Delta\eta_N)^2}\frac{\partial}{\partial\eta}\{\frac{\mu_{eff}}{\sigma_{t,\bar{h}}}(\sigma_{t,\bar{h}} - 1)\frac{\partial w^2/2}{\partial\eta}\} + \frac{1}{(\Delta\xi_E)^2}\frac{\partial}{\partial\xi}\{\frac{\mu_{eff}}{\sigma_{t,\bar{h}}}(\sigma_{t,\bar{h}} - 1)\frac{\partial w^2/2}{\partial\xi}\}$
f	$\frac{\mu_t}{\sigma_{t,\bar{f}}}$	0

Table (2),below, provides values for the laminar Prandtl, number, σ, and for the turbulent Prandtl number $\sigma_{t,\phi}$. Also given in Table (3) are values for the constants associated with the turbulence model: C_1 and C_2 which are required in the source term of the k and ε equations; C_D which is used to obtain the turbulent viscosity as will be described in Section (2.6) below, and K and E which are constants required in the law-of-the-wall formulation described in Section (3.4-4) below.

TABLE (2)

Values of the laminar and turbulent Prandtl numbers

ϕ	$\sigma_{t,\phi}$	σ
k	1.0	.7
ε	1.3	.7
$\tilde{h}$	.9	.7
f	.9	.7

TABLE (3)

Values of the constants in the turbulence model formulation

K	E	C_D	C_1	C_2
.42	9.0	.09	1.44	1.92

Previous experience of applying the above equations to a large number of flow situations, has revealed that these constants tend to be nearly universal constants. However, a "fine-tuning" of their values for each particular flow situation may be necessary to optimise the results.

2.5 Auxiliary Information

In addition to the partial differential equations, the complete specification of the mathematical problem requires provision of auxiliary information of four types:

- Inlet conditions, i.e. initial values of dependent variables corresponding to the position of the coordinate along the predominant flow direction, ζ, at which solutions to the set of equations are initiated;
- Boundary conditions, i.e. conditions of all the dependent variables at the E, W, N and S boundaries, as a function of ζ;
- Physical hypotheses which permit the calculation of diffusion coefficients as well as sources and sinks of each variable, in terms of the dependent variables of these equations, over the entire flow field; and
- Certain relationships among the thermodynamic and transport properties.

2.5-1 Inlet conditions

Information to start the marching integration is needed. This information must be provided as the inlet conditions of all dependent variables, fluid properties and the other auxiliary variables, at the plane at which solution is initiated. For the flows under consideration, this means specifying the velocities, pressures, enthalpies, species mass fractions, turbulence quantities and the physical properties, density, viscosity and specific heat.

Any type of uniform or non-uniform distributions at inlet may be specified and supplied to the calculation procedure in a simple manner. For example, a distribution of experimentally-determined velocities may be supplied as a function of grid position. So also may the static-pressure and temperature distributions.

2.5-2 Boundary conditions

Boundary conditions along the N, S, E and W surfaces (see Figure 4) must be specified for each variable. Any one of the above boundaries may be either (1) a symmetry plane, (2) a wall or (3) a free surface; and, as a consequence, different boundary conditions may apply on the different faces of the domain. These boundary conditions can be specified as the value of the variable ϕ or the flux of ϕ through the surface. A detailed discussion of boundary conditions is given in Section 3.4.3.

2.5-3 Physical hypotheses

- The gas density is calculated by the ideal-gas law, namely:

$$\rho = \frac{pW}{RT} \qquad ; \ (2.5\text{-}1)$$

where the mixture molecular weight W is calculated from:

$$\frac{1}{W} = \sum_j \frac{m_j}{W_j} \qquad ; \ (2.5\text{-}2)$$

where the summation is taken over all the chemical species j in the flow field. Details on the calculation and use of density in compressible-flow situations are given in Section 3.5.

- The laminar viscosity is taken into account only in the vicinity of walls, through the "wall functions" {6} to be described in Section 3.4-3. Its value is constant.

  There is no need for its inclusion in the core of such highly turbulent flows as the ones under study.

- The turbulent viscosity is determined by means of the k-ε model of turbulence employed. According to this model, the magnitude of the viscosity depends only on the local values of the turbulence kinetic energy k, on the dissipation rate of turbulence energy, ε, and on the fluid density, ρ. The turbulent viscosity is then given by:

$$\mu_t = C_D \rho k^2 / \varepsilon \qquad ; \ (2.5\text{-}3)$$

where C_D is a constant, given in Table 3.

The length scale in this model is obtained from:

$$\ell = C_D \frac{k}{\varepsilon}^{3/2} \qquad , \ (2.5\text{-}4)$$

and may be used for printing purposes, since its physical interpretation is more readily understandable than that of ε.

2.5-4 Thermodynamic and transport relationships

In order to calculate the fluid temperature and density, it is necessary to know the mass fraction of each chemical species at a given location.

Thermodynamic equilibrium is assumed so that the species mass-fraction distribution is calculated from the local temperature, pressure, and element fractions. Details of this technique are given in Appendix A.

Another important relationship is between the stagnation enthalpy and the temperature. This relationship is:

$$\bar{h} = \sum_j m_j h_j^o + \frac{u^2+v^2+w^2}{2} + C_p\,(T - T_{ref}) + k \qquad (2.5\text{-}3)$$

where C_p is the mixture specific heat and T_{ref} is the reference temperature for which the species enthalpy of formation, h_j is defined. Strictly speaking the right hand side of equation (2.5-3) should include the local kinetic energy of turbulence as an additional term. This term has been neglected here because it is many orders of magnitude lower than the other three terms for the flows considered. For the present work, T_{ref} is taken as 0^oK so that C_p is defined by:

$$C_p \equiv \frac{1}{T-T_{ref}} \int_{T_{ref}}^{T} C_p dT = \frac{h-h_{ref}}{T-T_{ref}} \qquad (2.5\text{-}4)$$

where h is the specific enthalpy at temperature T.

3. THE NUMERICAL ANALYSIS

3.1 Introduction

In this chapter, details are provided of a numerical scheme reported by Patankar and Spalding {7} for the solution of the mathematical problem described in Chapter 2. The layout of the rest of this chapter is as follows: Section 2 describes the procedures adopted in the discretization of equations (2.3-1) and (2.3-2). The computational structure of the numerical scheme employed is outlined in Section 3. In Section 4, the manner of incorporation of auxiliary information into the computational procedure, is briefly outlined. The treatment of compressibility is reported in Section 5 which closes the chapter.

3.2 The Discretization Procedure

The finite-difference equivalents of the differential equations are obtained by integrating the latter over the control volumes which surround the nodes of a grid system.

This procedure is described in the following sections.

3.2-1 The Grid system

The finite-difference grid used consists of:

(a) In the η-ξ planes, a system of intersecting, orthogonal grid lines of constant η and ξ. No restrictions are placed upon the spacing between the lines in any given direction.

(b) Planes of constant ζ at which solutions are obtained are arrived at by taking succesive increments (i.e. forward steps) along the ζ direction (main flow direction).

The limits on the size of the forward step, $\Delta\zeta$, are governed by considerations of stability and accuracy of the numerical procedure.

3.2-2 Storage locations

The intersections of the grid lines mentioned above are termed grid nodes. All the fluid properties with the exception of the velocity components u and v, are stored at the grid nodes. The velocity v is located midway between grid nodes in the η-direction, and velocity u similarly located along the ξ direction. Figure (5) illustrates this "staggered" grid system in the η-ξ plane. The boomerang-shaped envelopes shown on the figure enclose the triads of

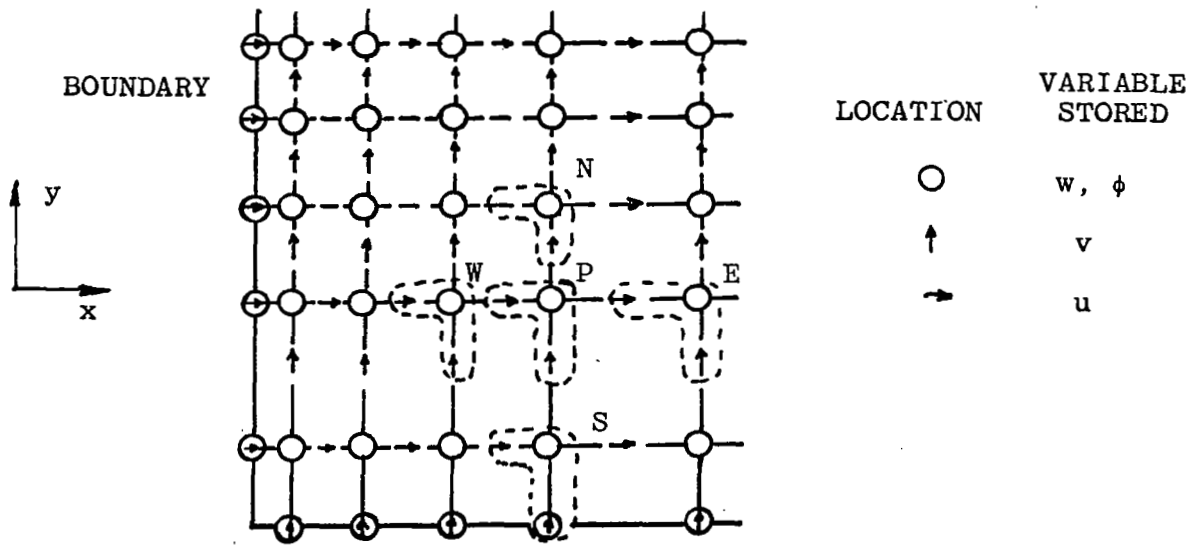


FIGURE 5: STAGGERED LOCATION OF VARIABLES

points denoted by the single letter, N,S,E,W or P, which represent a unique computer storage location.*

In the algebra connected with the discretization procedure, when a variable is required at points other than those at which it is located, averages of neighbouring values are used to arrive at the value of the variable at that point.

3.2-3 Control volumes

The control volume surrounding each grid node P, indicated in Figure {6} has two faces that coincide with two constant-ζ planes. One of these, at which integrations of the partial differential equations are to be performed, is designated the downstream (D) station. The other faces are midway between the nodes, so that the velocity components giving rise to convective fluxes along the η and ξ directions are located on the faces themselves.

Figure {7}, illustrates this point, with reference to a cross-section of the control volume in the ξ-η plane. It is over such control volumes, that balances of w, ϕ and mass are made in the calculation procedure. Similar control-volumes,resulting from the "staggering" of locations on the grid, are defined to surround the locations of the v and u velocity components. Three sets of control volumes are thus identifiable over the entire calculation domain.

A slight modification to the variable location and control-volume definitions is made in the region of boundaries of the calculation domain. The control volumes corresponding to the near-boundary velocities v in the case of N and S ,and u in the case of E and W boundaries, are arranged to extend right up to the boundary. Figure (8) illustrates this point.

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* Note on change in notation. N,S,E,W were used in Chapter 2 to denote domain boundaries. From here on they will denote neighbouring grid nodes.

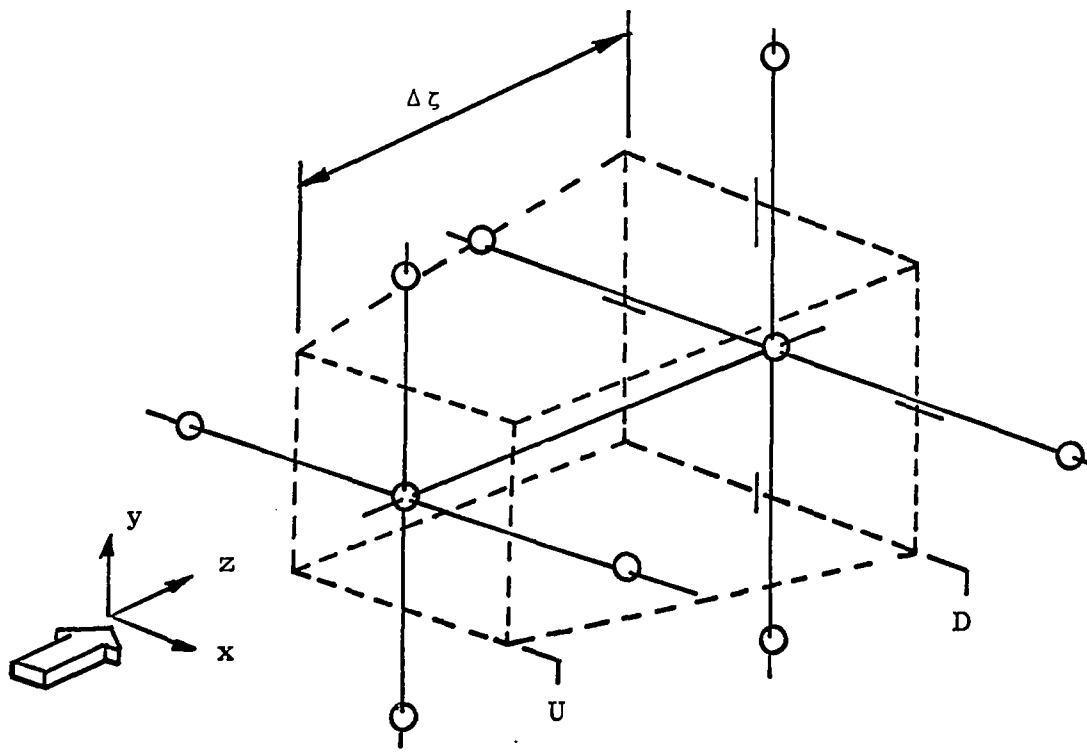


FIGURE 6: FINITE-DIFFERENCE CONTROL VOLUME

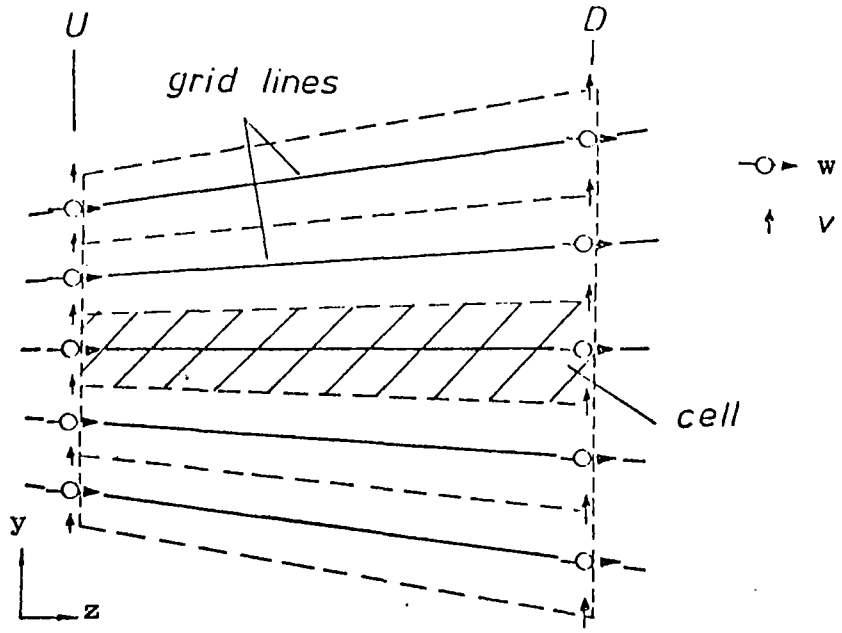


FIGURE 7: CONTROL VOLUME WHEN THE GRID EXPANDS TO ACCOMMODATE EXACTLY THE DIFFUSER SHAPE. NOTE THE INCLINATION OF THE w-VELOCITY ARROW WITH GRID LINES

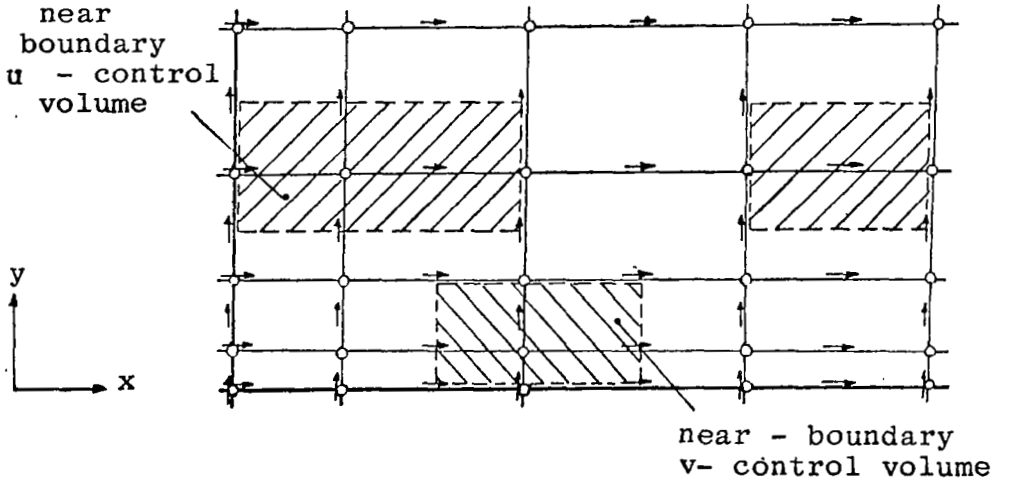


FIGURE 8: THE NEAR-BOUNDARY MODIFICATION TO CONTROL VOLUMES

3.2-4 The Discretized equation

The general discretized equation is obtained by integrating equation (2.3-2), for each variable, over the appropriate control volume. In the integration, the following assumptions are made about the manner in which the variables vary between grid nodes.

(a) In the z-direction, ϕ varies in a stepwise manner; i.e. the downstream values of ϕ are supposed to prevail over the interval from the upstream station to the downstream one except at the upstream station itself. This makes the present finite-difference scheme a fully-implicit one.

(b) For the calculation of the z-direction convection, and of source terms that may depend on ϕ, the variation of ϕ in the xy-plane is also taken to be stepwise. Thus, in the xy-plane the value of ϕ is assumed to remain uniform and equal to ϕ_P over the control volume surrounding the point P and to change sharply to ϕ_N, ϕ_S, ϕ_E, or ϕ_W outside this control volume.

(c) For the cross-stream convection from the yz and xz faces of the control volume, the value of ϕ convected is taken to be the arithmetic mean of the ϕ values on either side of that face, except when this practice is altered by the "high-lateral-flux" modification mentioned below.

(d) For diffusion across the yz and xz faces of the control volume, we assume that ϕ varies linearly between grid points, except when the high-lateral-flux modification dictates otherwise.

The result of these operations is an algebraic equation for each grid location, representing the discretized form of the balance of the variable, over the control volume corresponding to that location. For a general dependent variable ϕ, this equation takes the form:

$$\begin{aligned} & L^{\zeta}{}_{P}\phi_P - L^{\zeta}_{P,U}\,\phi_{P,U} + f_n L^{\eta}_n\,(\phi_N + \phi_P) - f_s L^{\eta}_s(\phi_P + \phi_S) \\ & + f_e\,L^{\xi}_e\,(\phi_E + \phi_P) - f_w\,L^{\xi}_w\,(\phi_P + \phi_W) = S_P{}^{\phi} \\ & + T^{\eta}_n\,(\phi_N - \phi_P) - T^{\eta}_s\,(\phi_P - \phi_S) \\ & + T^{\xi}_e\,(\phi_E - \phi_P) - T^{\xi}_w\,(\phi_P - \phi_W) \end{aligned} \qquad (3.2\text{-}1)$$

The factors f_e, f_w, f_n, and f_s are interpolation factors to account for the staggered cells. For the ϕ cells, they are all 0.5.

Attention is drawn here to the manner of discretization of the convective terms in the η- and ξ directions. The method used is designated the "high-lateral-flux modification" and is discussed in detail in {8}. It is briefly described later.

The coefficients of equations (3.2-1) are now defined as follows:

$$L^{\zeta}_{P,U} = (\rho w)_{P,U}\ \Delta\xi_P \Delta\eta_P \Delta\xi_E \Delta\eta_N \qquad (a)$$

$$L^{\eta}_{j} = \left[\rho v - \rho w \left\{\frac{d}{dz}(\Delta\eta_S) + \eta\frac{d}{dz}(\Delta\eta_N)\right\}\right]_j \Delta\xi_P \Delta\zeta \Delta\xi_E \qquad (b)$$

$$L^{\xi}_{i} = \left[\rho u - \rho w \left\{\frac{d}{dz}(\Delta\xi_W) + \xi\frac{d}{dz}(\Delta\xi_E)\right\}\right]_i \Delta\eta_P \Delta\zeta \Delta\eta_N \qquad (c)$$

$$L^{\zeta}_{P} = L^{\zeta}_{P,U} - L^{\xi}_{e} + L^{\xi}_{w} - L^{\eta}_{n} + L^{\eta}_{s} \qquad (d)$$

$$T^{\xi}_{i} = \Gamma_{\phi,i}\frac{\Delta\eta_P \Delta\zeta \Delta\eta_N}{\delta\xi_i \Delta\xi_E} \qquad (e) \qquad (3.2\text{-}2)$$

$$T^{\eta}_{j} = \Gamma_{\phi,j}\frac{\Delta\xi_P \Delta\zeta \Delta\xi_E}{\delta\eta_j \Delta\eta_N} \qquad (f)$$

$$S^{\phi}_{P} = S_{\phi,P}\Delta\xi_P \Delta\eta_P \Delta\zeta\, \Delta\xi_E \Delta\eta_N \qquad (g)$$

where,

Δ's and δ's represent the widths of control-volume faces and internodal distances respectively (see Figure 9), and i and j stand for locations (e,w) and (n,s) respectively.

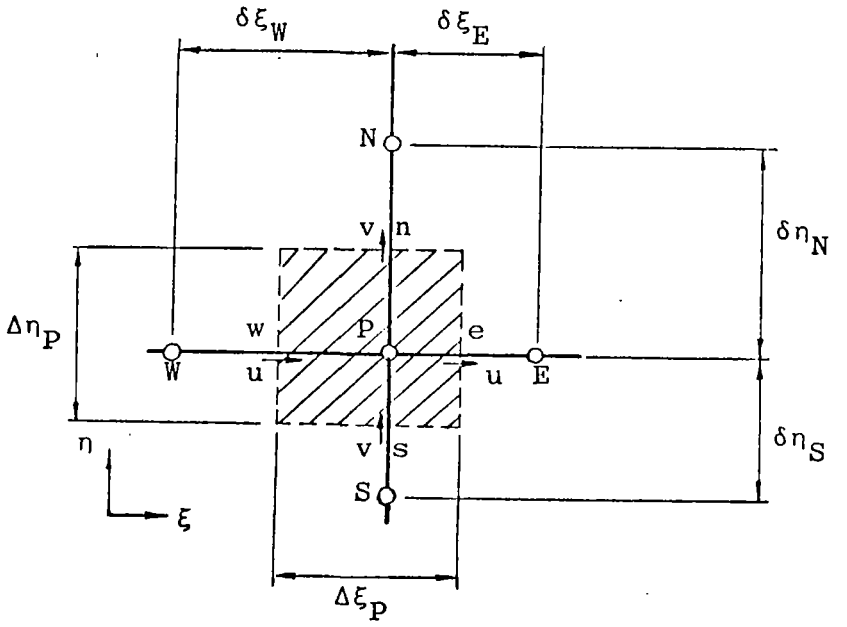


FIGURE 9: GRID NOMENCLATURE FOR DISCRETIZATION PROCEDURE

$\Delta\zeta$ is the forward step size, and S_P^{ϕ} is the integrated form of the source (and/or sink) of ϕ, always expressed for reasons of numerical stability in a linearised form as:

$$S_P^{\phi} = S_U + S_P \phi_P \qquad (3.2\text{-}3)$$

Where S_U and S_P are calculated from values already in computer store at that time. Expressing source terms in linearised form enhances the stability of the finite-difference equations, and is recommended as a useful practice to be applied wherever possible. Further it is also necessary that S_P be negative always if stability is to be ensured.

On re-arranging the terms of equation (3.2-1), one obtains:

$$\Sigma A_i' \phi_P = \Sigma A_i' \phi_i + S_P^{\phi} \qquad (3.2\text{-}4)$$

$i = N,S,E,W,U \qquad i = N,S,E,W$

where the coefficients A_i' are defined as follows:-

$$A_E' = T_e^{\xi} - \frac{1}{2} L_e^{\xi} \qquad (a)$$

$$A_W' = T_w^{\xi} + \frac{1}{2} L_w^{\xi} \qquad (b)$$

$$A_N' = T_n^{\eta} - \frac{1}{2} L_n^{\eta} \qquad (c)$$

$$A_S' = T_s^{\eta} + \frac{1}{2} L_s^{\eta} \qquad (d) \qquad (3.2\text{-}5)$$

$$A_U' = L_{P,U}^{\zeta} \qquad (e)$$

$$S_P^{\phi} = (S_U + S_P \phi_P) + L_{P,U}^{\zeta} \phi_{P,U} \qquad (f)$$

where the L's represent convective contributions, T's the diffusive and S the source (and/or sink) contributions to the balance of ϕ.

The subscripts are associated with points on the grid system and superscripts to the co-ordinate directions for which the coefficient is appropriate. The location of points e,w,n,s, E,W,N,S is given in Figure (9).

Note that in the derivation of A_i', account has been taken of the fact that the faces of the main control volumes pass midway between grid nodes so that the interpolation factors for the calculation of variables on these faces are equal to 0.5. This is not true for the control volumes appropriate to u- and v- velocity components in the general case of non-uniform spacing between grid nodes. Direct interpolation is then necessary so that the value of u at point P is given by:

$$f_e \, u_E + f_w \, u_P$$

and similarly for v. Note also that: $f_w = 1 - f_e$

It is possible for the convective contribution L_j^i of the coefficient A' to become large on occasion, resulting in the coefficient becoming negative and causing physically implausible results when equation (3.2-4) is solved with such coefficients. The high-lateral-flux-modification, mentioned above, is introduced to overcome this possibility. This scheme consists of replacing all the coefficients of the form T_j^i by $\bar{T}_j^i$ as follows:

$$\bar{T}_j^i \equiv \frac{1}{2}\left[T_j^i + \left|\tfrac{1}{2}L_j^i\right| + \left| T_j^i - \left|\tfrac{1}{2}L_j^i\right| \right| \right] \qquad (3.2\text{-}6)$$

where $|A|$ signifies the modulus of A.

3.2-5 Equations for velocity components

The finite-difference equations for the velocity components are described by the same form as (3.2-4) but contain an additional source term representing the pressure-gradient. Since we shall be using the velocity equations later in deriving the continuity balance, it is necessary to note here their form.

ζ-direction momentum equation

$$w_P = \sum_{i=E,W,N,S} A_i^w w_i + S_P^w + D_P^w \frac{\partial \bar{p}}{\partial \zeta} \qquad (3.2\text{-}7)$$

η-direction momentum equation

$$v_P = \sum_{i=E,W,N,S} A_i^v v_i + S_P^v + D_P^v (p_P - p_S) \qquad (3.2\text{-}8)$$

ξ-direction momentum equation

$$u_P = \sum_{i=E,W,N,S} A_i^u u_i + S_P^u + D_P^u (p_P - p_W) \qquad (3.2\text{-}9)$$

where,

A_i^ϕ denotes again coefficients of the form:

$$A_i^\phi = \frac{A_i'^\phi}{\sum_{i=E,W,N,S,U} A_i'^\phi} \qquad (3.2\text{-}10)$$

where ϕ now stands for u, v and w*

$$D_P^w = -\Delta\zeta\Delta\eta_P\Delta\xi_P\Delta\eta_N\Delta\xi_E \quad , (a)$$
$$D_P^v = -\Delta\zeta\Delta\xi_P\Delta\xi_E \quad , (b) \qquad (3.2\text{-}11)$$
$$D_P^u = -\Delta\zeta\Delta\eta_P\Delta\eta_N \quad , (c)$$

and,

S_P^ϕ represents the source (and/or sink) of each velocity excluding the pressure-gradient terms.

The pressure term employed in the w-equation depends on whether the local flow is subsonic or supersonic. When the flow is subsonic, it is necessary, {7}, in order to render the equations parabolic, to write the source term as a mean pressure gradient, i.e.,

$$S_w = \frac{\partial \bar{p}}{\partial \zeta} = \frac{\bar{p} - \bar{p}_U}{\delta\zeta} \qquad (3.2\text{-}12)$$

---

*Note that these A_i's now relate to the staggered control volumes described earlier.

where $\bar{p}$ denotes the mean pressure which is determined for a confined flow from the requirements of overall continuity; for an unconfined flow, $\bar{p}$ is simply the free-stream pressure. For a supersonic flow in contrast, it is possible, without destroying the parabolic nature of the equations, to employ the local pressure to calculate the pressure gradient, i.e.,

$$S_w = \frac{\partial p}{\partial \zeta} = \frac{p_P - p_{P,U}}{\delta \zeta} \qquad (3.2\text{-}13)$$

This practice, it should be observed, allows full account to be taken of pressure waves in supersonic flow.

3.2-6 The continuity equation

The derivation of the finite-difference form of the continuity equation is quite simple. It merely states the requirement that the inflows and outflows of mass are locally in balance at all the grid nodes in the flow domain. In the present solution procedure, the requirement of mass continuity is satisfied by correcting the pressure field via a pressure-correction equation. The details of the latter will be given in Section 3.3 below; here we state merely the requirement of continuity as follows:

continuity

$$\{G_e^{\xi} - G_w^{\xi}\}\ \Delta\eta_P \Delta\zeta\ \Delta\eta_N + \{G_n^{\eta} - G_s^{\eta}\}\ \Delta\xi_P \Delta\zeta\ \Delta\xi_E =$$

$$\{G_{P,U}^{\zeta} \Delta\eta_{P,U} \Delta\xi_{P,U} \Delta\eta_{N,U} \Delta\xi_{E,U} - G_P^{\zeta} \Delta\eta_P \Delta\xi_P \Delta\eta_N \Delta\xi_E\} \qquad (3.2\text{-}14)$$

where,

G_i^j represents the mass velocity along direction j atlocation i. For example:

$$G_s^{\eta} = (\rho v)_s - \left[\rho w \{\frac{d\Delta\eta_s}{dz} + \eta \frac{d}{dz}(\Delta\eta_N)\}\right]_s \qquad (3.2\text{-}15)$$

$\Delta\eta_{P,U}$ and $\Delta\xi_{P,U}$ represent the upstream values of $\Delta\eta_P$ and $\Delta\xi_P$ respectively.

It should be noted here that two distinct densities are computed and used at each step. The downstream density (ρ_P) is used only to compute the mass flux in the ζ direction at the downstream face of the cell (thus it appears only in the last term of equation (3.2-14); the upstream density ($\rho_{P,U}$) is used for calculating lateral mass fluxes, and the upstream axial mass flux. The two densities are calculated as follows:

$$\rho_P = \frac{p_P W_{P,U}}{RT_{P,U}} \qquad (3.2\text{-}16)$$

$$\rho_{P,U} = \frac{p_{P,U} W_{P,UU}}{RT_{P,UU}} \qquad (3.2\text{-}17)$$

where W_P is the local mixture molecular weight, R is the universal gas constant, and subscript 'UU' refers to the plane two steps upstream of the plane in question.

3.3 The Solution Procedure

3.3-1 The computational algorithm

The above set of finite-difference equations has to be solved for all the variables simultaneously, at the downstream station. After completion of the solution at the downstream station, a forward step in the ζ-direction is taken and the procedure repeated.

The numerical algorithm embodied in SHIP is the SIMPLE (for Semi-Implicit Method for Pressure-Linked Equations) scheme reported earlier in {7} by Patankar and Spalding. Central to this scheme is the idea of seeking a non-iterative marching-integration procedure that takes full advantage of the boundary-layer character of the flow field.

At each axial location the variables are computed solely from values at the upstream location; no reference is made to downstream properties. Further, the coefficients (A's) used in the equations are evaluated from the values currently in store; for the velocities, this means use of the upstream values. The sequence of calculation steps to evaluate the flow properties at any axial station is as follows:

1) First the pressure field p and the mean pressure $\bar{p}$ at the axial station considered are assigned 'guessed' values. The general practice is to employ the calculated upstream pressures as the guessed values and to estimate $\bar{p}$ using the upstream pressure gradient $d\bar{p}/dz$.

2) The three momentum-equations are solved to get a first approximation to the velocity field at the longitudinal station.

3) The resulting "starred" velocity field is used in conjunction with the discretized continuity equation to arrive at a distribution of "pressure-corrections" p' as follows.*

(a) First the pressure and velocity fields are expressed as:

$$\begin{aligned} p &= p^* + p' \\ u &= u^* + u' \\ v &= v^* + v' \end{aligned} \qquad (3.3\text{-}1)$$

where the primed quantities represent the corrections to the approximate *starred* values. The latter will not, in general, satisfy the continuity equation, but will give rise to a net mass source at P.

(b) It is now required to obtain the corrections to the velocities and pressures so as to reduce this mass source to zero. To this end, the substitution of equation (3.3-1) into the momentum equations results in the following expressions:

$$\begin{aligned} u'_P &= \Sigma A_i^u u'_i + D_P^u (p'_P - p'_W) \\ v'_P &= \Sigma A_i^v v'_i + D_P^v (p'_P - p'_S) \end{aligned} \qquad (3.3\text{-}2)$$

where the summation Σ is carried out over the grid nodes neighbouring the corresponding velocity.

---

*Readers not interested immediately in the details of the pressure-correction equation may skip to step 4, but should note that the pressure-correction equation has the same general structure as that of (3.2-4), and that it is solved in the same manner as the others.

(c) The relations expressed above are substituted in the finite-difference form of the continuity, equation (3.2-14); and the coefficients for p'_P are collected and rearranged. The pressure correction equation has then the following form:

$$p'_P = \sum_{i=E,W,N,S} A_i^{p'} p'_i + S_P^{p'} \qquad (3.3\text{-}3)$$

where p'_E, p'_W, p'_N and p'_S are corrections to the pressures at the nodes E,W,N and S, the A_i's involve ρ's, D's and other geometric quantities appearing in equation (3.2-14), and the mass source, (or mass imbalance) has been incorporated into $S_P^{p'}$.

For compressible flow, account must be taken of the effect of a pressure change at P on the mass flux at the downstream face of the cell. Thus for supersonic flow the mass-flux change $(\rho w)'_P$ is related to the pressure correction p'_P by:

$$(\rho w)'_P = \{\rho^*_P D_P^W + (\frac{d\rho}{dp})_P w_P^*\} p'_P \qquad (3.3\text{-}4)$$

where, ρ^*_P and w^*_P are computed from the guessed pressure p^*_P; $(d\rho/dp)_P$ is, from equation (3.2-16)

$$(\frac{d\rho}{dp})_P = \frac{W_{P,U}}{RT_{P,U}} \qquad (3.3\text{-}5)$$

$$\text{and} \quad D_P^W = \frac{w'_P}{p'_P} \qquad (3.3\text{-}6)$$

and is deduced from the finite-difference form of the momentum equations.

For subsonic flow, equation (3.3-4) must be modified to account for the fact that w_P no longer depends on p_P; the modified expression is:

$$(\rho w)'_P = (\frac{d\rho}{dp})_P w^*_P p'_P \qquad (3.3\text{-}7)$$

(d) Equation (3.3-3), with the coefficients modified to account for the above-described influences of p'_P on $(\rho w)_P$, is solved in the same manner as the momentum equations. The resulting pressure-corrections are then used in correcting the pressure and velocity fields simultaneously.

4) The equations for the remaining variables (i.e. enthalpy, turbulent energy and its dissipation rate, and mass fraction of hydrogen in any form) are then solved, by using the corrected velocity fields.

Steps 1 - 4 complete the operations at a given downstream station. A new step is then taken and the process repeated, until the region of interest is covered.

3.3-2 The solution of the equations

The linear algebraic equations are solved by performing repetitive sweeps of the tri-diagonal matrix algorithm (TDMA) along the two cross-stream directions η and ξ. The equations are solved along lines of constant η and of constant ξ, and in doing so, the variables located at adjacent lines are kept constant. Thus for the η-direction sweep we have:

$$\phi_P = A'_N\phi_N + A'_S\phi_S + (A'_E\phi_E + A'_W\phi_W + S_P^\phi) \qquad (3.3\text{-}8)$$

where the terms enclosed in the parentheses are assumed to be fixed. Similarly, for the ξ-sweep we have:

$$\phi_P = A'_E\phi_E + A'_W\phi_W + (A'_N\phi_N + A'_S\phi_S + S_P^\phi) \qquad (3.3\text{-}9)$$

where now the values of ϕ_N and ϕ_S are kept fixed. The terms contained in S_P^ϕ however, are always like the A coefficients, evaluated from variables in store before the TDMA sweeps.

The number of TDMA sweeps required to obtain an accurate solution to the equations depends on the equation being solved. It has been found from experience that for the pressure-correction equation it is necessary to perform more sweeps than for the rest. The reason for this increase is as follows. The equation for a general variable ϕ is dominated strongly by the contribution from upstream (i.e. the term $L_{P,U}^{\zeta}\phi_{P,U}$ in equation (3.2-5 (f)). Therefore the coefficients A'_N, A'_S etc. are relatively small, and use of somewhat approximate values for ϕ_N, ϕ_S etc. does not result in significant errors. For the pressure-correction equation however, there is no contribution from upstream, and the pressure correction at P is related strongly to

the N,S,E and W values. It is therefore necessary to perform several sweeps to obtain accurate values.

3.4 Boundary Conditions

3.4-1 The solution domain

SHIP is set up to make calculations in a rectangular-sectioned domain of any aspect ratio. The boundaries of this domain may be either solid walls, symmetry planes or free boundaries; and indeed any combination of the above boundaries can be handled. Furthermore, for walls, the distance of each wall from a reference plane can be specified as an arbitrary, but smooth, function of distance along the principal flow direction.

In the region of free-boundaries the flow is unconfined and expands as it proceeds downstream. Two considerations must, therefore, be taken into account here, namely the prescription of the rate of expansion of the solution domain and the specification of the mass velocities at the outer free-boundary. The latter will be described in Section 3.4-3 below.

For the former, a slope of the boundary is prescribed; and if this leads to solution showing excessive velocity and temperature gradients the calculation is repeated by moving the free-boundaries outwards or changing the slope of the free surface in the desired direction to diminish gradients.

3.4-2 General policy of treating boundaries

The SHIP program requires the specification of boundary conditions on the N, S, E and W boundaries to ξ - η planes of the calculation domain.

A clear distinction is made, for all dependent variables, between boundary values and values internal to the domain. The main machinery of the program leaves the boundary values unchanged, although it uses them in determining the internal values. Thus, the procedure is so structured that it nominally solves the fixed-boundary-value problem. When boundary values are not known however, appropriate modifications are devised which permit the single structure to be used. The following sections describe such modifications.

In general, boundary-condition information can be supplied to the numerical calculation procedure in one of four ways. The boundary values of the dependent variables themselves can be modified; or the values of Γ at the boundary nodes can be suitably adjusted. Alternatively, the source terms for the near-boundary control volumes or the finite-difference coefficients themselves can be suitably modified. SHIP is

equipped with source-term modification practices.

3.4-3 Treatment of the types of boundaries handled by SHIP

SHIP allows for any of the four boundaries to be (1) a symmetry plane (2) a wall, or (3) a free surface.

(1) Treatment of symmetry planes

At symmetry planes and at the axis of symmetry, the velocities normal to the boundary are zero; and there are no fluxes across them of other flow variables. In the present solution scheme such boundary conditions are incorporated as follows. The normal velocities at these boundaries are prescribed to be zero a priori and not altered; for other variables, because both the convective and diffusive fluxes are zero, the appropriate finite-difference coefficients connecting the boundary node to the near-boundary one are set to zero, thus breaking their links.

(2) Treatment of wall boundaries

a) At solid walls, all the three components of velocity are zero and are prescribed a priori. For turbulent kinetic-energy, k, and its dissipation rate, ε, the boundary-conditions are prescribed through wall functions described below; no reference is made to the values of k and ε on the wall nodes. The values of k and ε on the wall therefore, are prescribed arbitrarily to be zero, and have no influence on the solution scheme. For enthalpy, the SHIP code provides the choice between specification of an adiabatic wall or a constant temperature one, for each wall. In the former case, (prescribed zero-flux boundary condition), the value stored as wall temperature does not enter the calculations.

In the region close to the wall, the correct fluxes of momentum are calculated through wall functions described below.

b) Wall functions

The expressions for Γ appropriate to turbulent flow are not strictly valid in the vicinity of wall boundaries to the flow, where laminar viscosity plays an important rôle. If the near-boundary grid nodes are sufficiently far away from walls, the turbulent viscosity can continue to be used for internal grid nodes. However, means must be provided for calculation of the correct shear stresses as well as fluxes of other dependent variables at the wall boundaries.

Provisions for such calculations are made in the program, and use the so-called wall-function concept. In this concept, the flux of a variable ϕ at a wall boundary, is expressed as:

$$\phi''_{wall} = \Gamma_{\phi,wall} \frac{\phi_{near\ wall} - \phi_{wall}}{\delta_{wall}} \qquad (3.4\text{-}1)$$

where δ_{wall} denotes the normal distance from the wall to the near-wall point. Values of $\Gamma_{\phi,wall}$ are obtained from the presumption that in the region adjacent to wall boundaries, the dependent variables obey, for turbulent flow, a modified form of the semi-logarithmic law-of-the-wall. The formulae used to calculate $\Gamma_{\phi,wall}$ are provided in Table (4).

TABLE 4. Diffusion Coefficient Formulae

ϕ	$\Gamma_{\phi,\ wall}$
Velocity components normal to the wall	0
Velocity components parallel to the wall	$y^+ > 11.5 : \dfrac{\mu y^+}{\frac{1}{K}\,\ell n\,\{Ey^+\}}$ $\leq 11.5 : \mu$
κ	0
ε	--
All other ϕ's (only for $\bar{h}$ in SHIP)	$y^+ > 11.5: \dfrac{\mu}{\sigma_{t,\phi}} \dfrac{y^+}{(\frac{1}{K}\,\ell n\,\{Ey^+\} + P_\phi)}$ $< 11.5: \dfrac{\mu}{\sigma}$

The definition of y^+, in the table, is a generalization due to Spalding {8} of the conventional form, in that:

$$y^+ = \frac{\rho C_D^{\frac{1}{4}} k^{\frac{1}{2}} \delta}{\mu} \qquad (3.4\text{-}2)$$

where δ denotes the distance from the wall, at a location with which the values of ρ and k are associated. The constants K and E are obtained from the conventional form of the law-of-the-wall:

$$u^+ = \frac{1}{K} \ell n \{E y^+\} \qquad (3.4\text{-}3)$$

and are given values of 0.42 and 9.0 respectively.

The boundary conditions of k and ε are provided as follows:

The diffusion of kinetic energy k, to the wall is known to be negligible and is set to zero and a balance equation for k, regular in other respects, is solved for control volumes adjacent to wall boundaries. The diffusion of dissipation rate ε to such boundaries is more difficult to express. Instead of the attempt to calculate $\Gamma_{\varepsilon,\text{wall}}$, use is made of the knowledge that the length scale ℓ varies linearly with distance from the wall, in the neighbourhood of the wall. The dissipation rate is then calculated from this length scale from:

$$\varepsilon_{\text{near wall}} = C_D^{\frac{3}{4}} \frac{k}{K\delta}^{3/2} \qquad (3.4\text{-}4)$$

The practice adopted is to fix $\varepsilon_{\text{near wall}}$ to the above value, without disturbing the general calculation procedure, in the following manner:

$$S_U^{\varepsilon} = L\, \varepsilon_{\text{near wall}} \quad (a)$$
$$S_P^{\varepsilon} = -L \quad (b) \qquad (3.4\text{-}5)$$

where L is a large number, say 10^{30}.

The expression for $\Gamma_{\phi,wall}$ for a general dependent variable ϕ is based on the expression indicated in Table (4), the value of P_ϕ being calculated from:

$$P_\phi = 9.24 \left[\frac{\sigma_\phi}{\sigma_{t,\phi}} - 1 \right] \left[\frac{\sigma_\phi}{\sigma_{t,\phi}} \right]^{-\frac{1}{4}} \qquad (3.4\text{-}6)$$

where σ_ϕ and $\sigma_{t,\phi}$ denote the laminar and turbulent values of Prandtl/Schmidt number appropriate to the transport of ϕ. The above equation is used in SHIP only for heat transfer.

3. Treatment of free-stream boundaries in supersonic flow

When the free-stream is supersonic, the velocities normal to a free-stream boundary can be deduced from the following equation:

$$v = \frac{p - p_\infty}{\rho_\infty w_\infty} \sqrt{M_\infty^2 - 1} \qquad (3.4\text{-}7)$$

where: $M_\infty = \rho_\infty w_\infty^2 / \gamma p_\infty \qquad (3.4\text{-}8)$

and ∞ denotes undisturbed free-stream conditions.

The above equation is based on the assumption that all changes to the lateral velocities, from their free-stream value along the free-boundary, have been brought about by a succession of small waves emanating from the viscous region. It has been programmed to compute the lateral boundary velocities, normal to the free boundary under consideration (i.e. the v-component for the North and South boundaries, and the u-component for the East and West ones.

Note that:

1. The formula is valid only for $M_\infty > 1$
2. The formula assumes v_∞ and u_∞ equal to zero
3. In the computer program, p in (3.4-7) is actually, p_{nb}, where nb denotes values at the near-boundary grid point.

4. The density at the boundary node is calculated from p_{nb}, but otherwise from conditions at ∞.

The formula holds true whether fluid is caused by the pressure changes to leave or enter the free boundary. If fluid enters, its stagnation enthalpy should be that of the free stream.

The longitudinal boundary velocity is calculated from the following equation derived from isentropic considerations:

$$w_b = \sqrt{w_\infty^2 + 2 \frac{\gamma}{\gamma-1} \frac{p_\infty}{\rho_\infty} \{1-(\frac{p_b}{p_\infty})^{\frac{\gamma-1}{\gamma}}\} - v_b^2 - u_b^2} \qquad (3.4\text{-}9)$$

where the subscript b denotes values at the boundary.

The derivation of equations (3.4-7) and (3.4-9) is given in Appendix B.

4. A DESCRIPTION OF THE COMPUTER PROGRAM

4.1 Introduction

In this chapter an overview of SHIP is given with a description of the program flow and control, and definitions of important variables.

4.2 General Structure

The general structure of the SHIP computer program is shown in Figure (10). The divided, vertical box on the left is the main program, MAIN, which has the chief function of controlling the calling sequence of the subprograms. The starting point for SHIP is at the top of this box. Points where calls of subprograms are made in SHIP are denoted by horizontal lines. Arrows indicate the "flow" of the computer program to and from the subprograms which are shown in boxes. The major calculations and logical decisions made by SHIP are indicated in the spaces between the horizontal lines marking calling points in SHIP.

The subprograms are contained in subroutines which are not individually called; and all start with an ENTRY statement. The subroutines are therefore never "called" by their names, but by the name of the appropriate member subprogram. (Thus CALL AUX is meaningless; but CALL SOURCE is a correct statement). No subprogram has any argument; the information is everywhere transferred through COMMON.

The SHIP program consists of 8 subroutines; they are given the names BLOCK DATA, MAIN, ALLMOD, AUX, PRINT, SOLVE, STRIDA and STRIDB. These subroutines can be classified in three categories: problem-dependent, physical-modelling-dependent and invariant. BLOCK DATA and ALLMOD are the problem-dependent routines, i.e. they provide for specification of inlet conditions, boundary conditions, geometry, fluid properties. etc. AUX forms the physical-modelling section of the program; in this the auxiliary quantities such as density and viscosity are calculated from physical laws and from the turbulence model. SOLVE, STRIDA, STRIDB and PRINT are the invariant portions of the program; in SOLVE, STRIDA and STRIDB, the calculation steps of section 3 are programmed, and in PRINT, instructions are provided to print out the distributions of the flow variables.

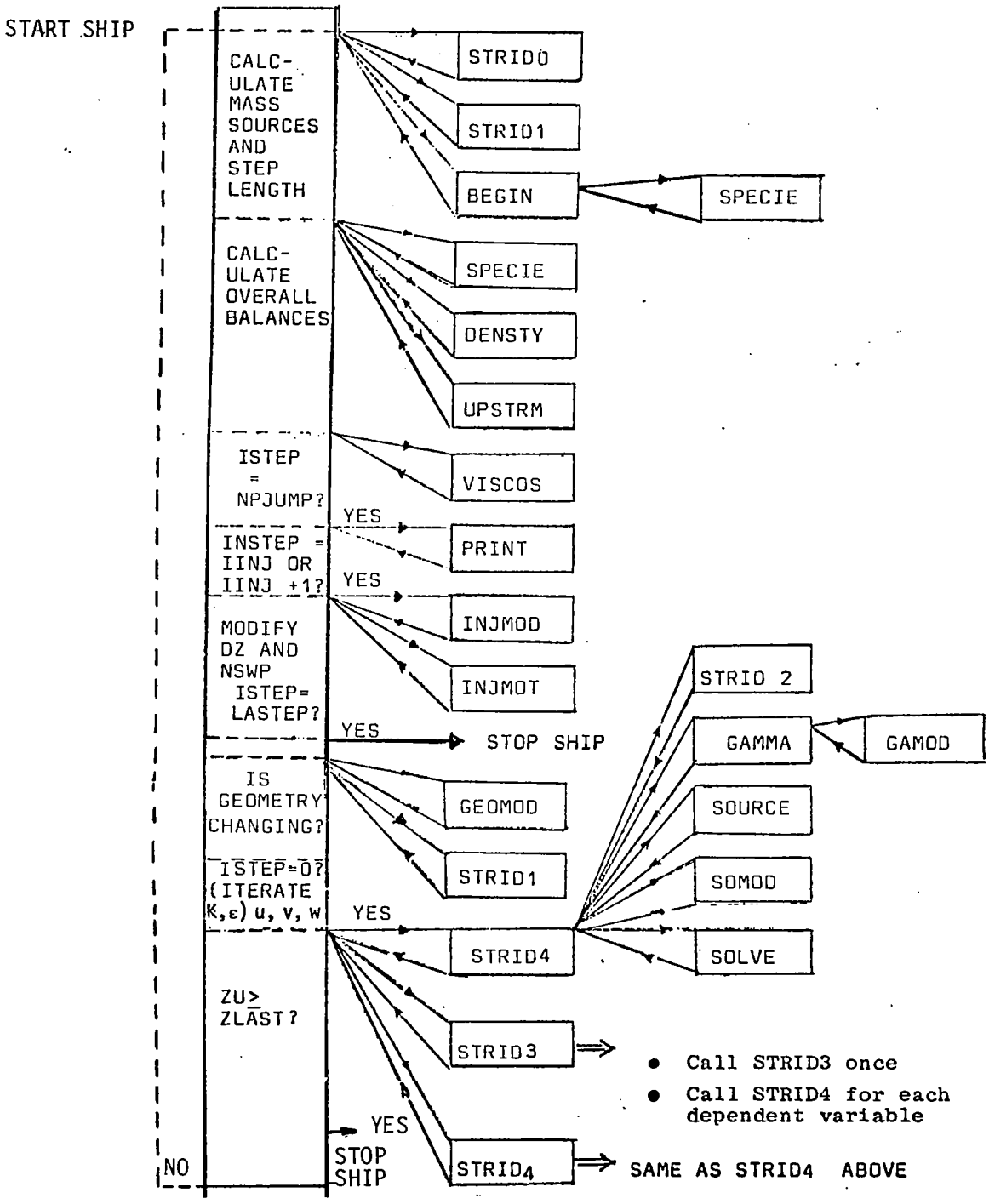


FIGURE 10: GENERAL STRUCTURE OF SHIP COMPUTER PROGRAM

The subprogram MAIN does not fit neatly into any of these categories. It has a general (i.e. problem dependent) structure, but care is necessary to ensure that its general structure is kept intact. The routine MAIN first calls routines STRID0, STRID1 and BEGIN. Through these calls, the initial information of geometry, grid and inlet profiles is prescribed. A loop for forward steps is then started. In this, calls are made in sequence, to routines UPSTRM, DENSTY, VISCOS, GEOMOD, STRID3 and STRID4. By these calls, the variables u,v,w,k,ε and h at one downstream location are calculated. STRID3 and STRID4, in turn, call routines dealing with the physical modelling section AUX and the problem-oriented subroutines in ALLMOD. When the finite-difference equations are assembled, through calls to AUX and ALLMOD, SOLVE is called to perform the TDMA sweeps. STRID3 contains four sections each having identical calling sequences of routines placed under AUX and ALLMOD. STRID4 calls the same routines as called by individual sections of STRID3; and solves the equations for the scalar variables k, ε and h.

The remaining part of this chapter gives a general overview of the computer program while succeeding chapters detail the operation of each subroutine.

4.3 Some Programming Conventions and FORTRAN Equivalents of Main Variables

A few of the FORTRAN names used in SHIP, which will be required in the following sections, are introduced here. The dependent variables ϕ are stored in an array F, which it is convenient to consider as a three-dimensional array F (I,J,NV). Here I and J denote the location (respectively along the ξ and η directions) and NV identifies a particular variable. The three velocity components and the pressure-correction are included in the F array; however, for ease in understanding, separate arrays U,V,W and PP are also used and made equivalent to parts of F as follows:

$$\begin{aligned} U(I,J) &\equiv F(I,J,NVU) \\ V(I,J) &\equiv F(I,J,NVV) \\ W(I,J) &\equiv F(I,J,NVW) \\ PP(I,J) &\equiv F(I,J,NPP) \end{aligned} \qquad (4.3\text{-}1)$$

The identifiers NVU, NVV, NVW and NPP, also used to identify U,V,W and PP elsewhere in the program, are assigned values 2,3,4 and 1. The largest values of I,J and NV for which storage is provided in the program are denoted by IMAX, JMAX and NNV respectively and assigned values 12, 20 and 9.

Although two- and three- dimensional arrays have been mentioned above, the computer program formally uses one-dimensional arrays, whose subscripts are calculated each time they are required. Thus, F(I,J,NV) is referred to as F(IJNV), where:

$$IJNV = I + JM(J) + NFM(NV) \qquad (4.3\text{-}2)$$

the arrays JM and NFM being calculated once and for all from:

$$JM(J) = (J - 1) * IMAX$$
$$NFM(NV) = (NV - 1) * IMAX*JMAX \qquad (4.3\text{-}3)$$

Also W(I,J) is referred to as W(IJ) where

$$IJ = I + JM(J) \qquad (4.3\text{-}4)$$

The four neighbouring points of the location IJ, corresponding to the points of the compass are referred to as IJ$\underline{N}$, IJ$\underline{S}$, IJ$\underline{E}$ and IJ$\underline{W}$. These are calculated as:

$$IJN = IJ + IMAX$$
$$IJS = IJ - IMAX$$
$$IJE = IJ + 1 \qquad (4.3\text{-}5)$$
$$IJW = IJ - 1$$

It is easy to see that points further removed become:

$$IJ\underline{NE} = IJN + 1 \qquad (4.3\text{-}6)$$
$$IJ\underline{SW} = IJS - 1 \quad \text{etc.}$$

For a given problem, all members of the F array for which provision is available, may not be required to be solved for. Furthermore, some of these variables may be obtained from algebraic equations and not from solutions of the partial differential equations. To provide for these alternatives, use is made of an array ISOLVE(NV). For ISOLVE(NV) equal to zero, the differential equation is not solved; solution is obtained for values of ISOLVE(NV) greater than zero. It is left to the user to make further use of this facility.

Other arrays directly related to members of the F array are: IPRINT(NV), TITLE(K,NV), FLUXN(I,NV), FLUXS(I,NV), FLUXE(J,NV), FLUXW(J,NV). Values of F(IJNV) are printed out if IPRINT(NV) is equal to 1; otherwise a printout is not obtained.

FLUXN(I,NV), stores the fluxes of the variable NV, on the North boundary; the others correspond respectively to the South, East and West boundaries. TITLE(K,NV) with the integer K taking values 1 - 9, stores a 36 character alphanumeric title of the corresponding variable NV. This is used to identify the values of the variables in the printout.

The quantities k, ε, h, f, and T form the remaining variables of the F family. They are identified by the indices NVK, NVD, NVH, NVF and NVT respectively and occupy NV locations 5, 6, 7, 8 and 9 in the array F(IJ,NV). No equation is solved for T; however, it is convenient to store it at F(IJ,9). Quantities p, ρ and Γ are stored as P(IJ), RHO(IJ) and GAM(IJ). They are not members of the F array, but are included along with F in a COMMON statement, and immediately following it. They can therefore be referred to as the $(NNV + 1)^{th}$, $(NNV + 2)^{th}$ and $(NNV + 3)^{th}$ members of the F array, as indeed they are in subroutine PRINT. The integers NVP, NRO and NMU are used to identify them.

Although, in general, the values of Γ are different for each dependent variable, storage provision for only one set of Γ's is retained. Hence, at a given stage in the program, the GAM array contains the values of Γ, appropriate to the dependent variable under consideration.

Similarly, provision is made, for the retention of one set of coefficients of the finite-difference equation at a given stage. Thus, AXP(IJ), AXM(IJ), AYP(IJ) AYM(IJ) and AZP(IJ) respectively represent the coefficients A'_E, A'_W, A'_N, A'_S and A'_U in equation (3.2-4).

Similarly, SU(IJ) and SP(IJ) represent S_U and S_P respectively in equation (3.2-3). The quantities like D_P^u in equation (3.2-9) are stored as DU(IJ), there being similar arrays DV(IJ) and DW(IJ) for the corresponding quantities associated with the v- and w- momentum equations.

4.4 Program Control

Program Control, including start, internal monitoring and stop functions, is achieved through subroutine MAIN.

Using the information supplied through BLOCK DATA, the first part of MAIN calculates and assembles all the geometrical information about the grid system through calls to STRID0 and STRID1. Following this, in the same part, a call to BEGIN supplies the initial conditions for all the dependent variables. Having provided the starting conditions,

MAIN then enters the marching-integration loop.

This part begins with the statement: 6Ø CONTINUE. Next, mass sources (SUM), step length (DZ) and the location of the station for the new calculation (ZD), are determined. This is followed by calls to SPECIE, DENSTY and UPSTRM. SPECIE calculates the chemical specie composition from element compositions, temperature and pressure. DENSTY is another member of the physical-modelling subroutine AUX, wherein the fluid density ρ, is calculated. UPSTRM stores the upstream values of the axial mass-flow-rate (GZ(IJ)), of the pressure (PU(IJ)) and of the height and width of the calculation domain (BYNU and BXEU) required by the calculation procedure.

After calculating and printing the fluxes of the major F arrays to check their overall balances, a call is made to VISCOS which calculates the diffusion coefficients for momentum and modifies them properly to account for the presence of solid walls if necessary.

If ISTEP equals NPJUMP, profiles of variables specified by IPRINT(NV)=1 will be printed out through a call to print. Otherwise, only overall balance information and station location will be printed out.

The next section is for the calculation of the velocity and pressure fields. First a check is made to see whether injection through either or both North and South boundaries occurs. If this test is positive, a call is made to INJMOD (for the South boundary) and/or INJMOT (for the North boundary) which provide the appropriate boundary conditions through source terms. It should be mentioned here that no restriction is placed upon the relative simultaneous spacing of the North and South injectors. Next a check is made to determine whether the station for calculation is immediately downstream of injection. If this test is positive the number of sweeps on the pressure correction equation and the step length are modified to increase accuracy and stability of the program. The calculation is stopped at this point if ISTEP > LASTEP.

Next a check is made to determine whether the flow domain under consideration presents varying geometry with axial distance or not. If this is true (IARCH=2), a call is made to subroutine GEOMOD and STRID1, in order for the geometrical changes to be taken properly into account. If the domain of interest retains constant cross-section along the axial distance, the above two subroutines need not be called.

After this test, another is performed to determine whether any of the four boundaries (North, South, East and West) is a free-boundary. If this test is positive, the free-boundary conditions are incorporated. Namely, the program calculates here, for any free-boundary, the proper densities and velocities as dictated from the small-wave theory (for the lateral velocity components) and from the isentropic formula (for the axial velocity component). These formulas have been discussed in detail in Section 3.

Next a check is made to determine if ISTEP=0 which, if positive, results in an iteration on the hydrodynamic and turbulence equations to improve the starting profile.

After this series of tests, a call is made to STRID3 which yields the velocity and pressure fields. A call to STRID4 performs similar calculations for all other dependent variables.

Then the program calculates and prints out the local values of wall fluxes at every existing wall and their averages. Useful quantities calculated here include mean velocity and dynamic head, total areas, wall shear stresses, drag coefficients and Stanton numbers.

Finally the value of ISTEP is incremented and, depending upon a pre-determined criterion, calculations are continued for the next station or terminated. This criterion is the limiting value of the forward distance. If ZU < ZLAST, control is returned to a point in MAIN just after the CALL BEGIN statement, and the process repeated for the next station.

4.5 Detailed List of Program Variables

All variables used in common statements are defined in Appendix C. Variables which appear locally are defined by their use in the computer program and are not defined in this report.

5. THE INVARIANT PORTION OF SHIP

5.1 Introduction

Many of the calculations do not need changing for different boundary conditions, etc. In this chapter the function of the invariant portion of SHIP is given. Again, important variables are defined.

5.2 STRIDA

STRIDA consists of three separate sections which are called through ENTRY statements. STRID0 and STRID1, the first two, calculate quantities related to the grid arrangement. The information supplied to STRIDA through BLOCK DATA is LCV, MCV and ZETA(I), ETA(J). The former represent the number of ϕ-control volumes along the ξ and η directions; and the latter denote the grid disposition in non-dimensional coordinates.

Given the above information, STRID0, the first member subroutine of STRIDA, computes the maximum number of grid nodes in the I and J directions. This is done in the following sequence:

```
L   = LCV + 1
M   = MCV + 1
LP1 = L + 1
MP1 = M + 1
```

(5.2-1)

It is emphasized here that users must ensure that LP1 and MP1 are always less than or equal to IMAX and JMAX respectively. The latter represent the maximum dimensions of all variables in the respective directions and are given values accordingly in BLOCK DATA. Following the above sequence, the integer arrays JM and NFM are filled in accordance with equation (4.3-3).

The second member of STRIDA is STRID1. STRID1 is called once at the beginning from MAIN and never again if the calculation domain cross-section remains unchanged. For domains of axially-varying cross-sections it is, however, called at every step from MAIN. It is in STRID1 that the physical coordinates x and y are computed from the values of AGEOM, ETA and ZETA, as follows:

```
X(I) = ZETA(I)*BXE
Y(J) = ETA(J)*BYN
```

(5.2-2)

ETA(J) is initially calculated as:

$$\text{ETA(J)} = \text{ETA(J-1)} + \text{AGEOM**(J-2)*DELY} \qquad (5.2\text{-}3)$$

where:

$$\text{DELY} = \text{BYN*}\ (1.0 - \text{AGEOM})/(1.0 - \text{AGEOM**M}) \qquad (5.2\text{-}4)$$

Here, BXE and BYN represent the width and height of the calculation domain respectively ($\{X_E - X_W\}$ and $\{Y_N - Y_S\}$ respectively); as such, they are to be specified by the user in BLOCK DATA. It should be mentioned that any ETA distribution can be used; the distribution (5.2-3) is just an example; it makes use of a geometric series for specifying successive intervals between ETA's. Larger values of AGEOM result in the grid being "crowded" closer to the y = 0 surface.

The width and height of the calculation domain are allowed, in SHIP, to be varied with axial distance; their new values being calculated by the expressions:

$$\begin{aligned} \text{BXE} &= \text{BXEU} + \text{DBXEDZ*DZ} \\ \text{BYN} &= \text{BYNU} + \text{DBYNDZ*DZ} \end{aligned} \qquad (5.2\text{-}5)$$

where BXEU, BYNU represent the upstream (i.e. of previous station) values of BXE, BYN and the quantities DBXEDZ, DBYNDZ (i.e. the slopes of BXE and BYN respectively) are specified by the user.

The ratio of cell areas in the ξ-η plane between upstream and downstream stations is also calculated in STRID1, and stored as ARAT; the expression for this ratio is:

$$\text{ARAT} = (\text{BYNU*BXEU})/(\text{BYN*BXE}) \qquad (5.2\text{-}6)$$

The subsequent operations in STRID1 deal with calculation of various inter-grid distances required later in the calculation of the coefficients. These distances are shown in Figure (11), which illustrates the grid in the η-ξ plane and the nomenclature described below.

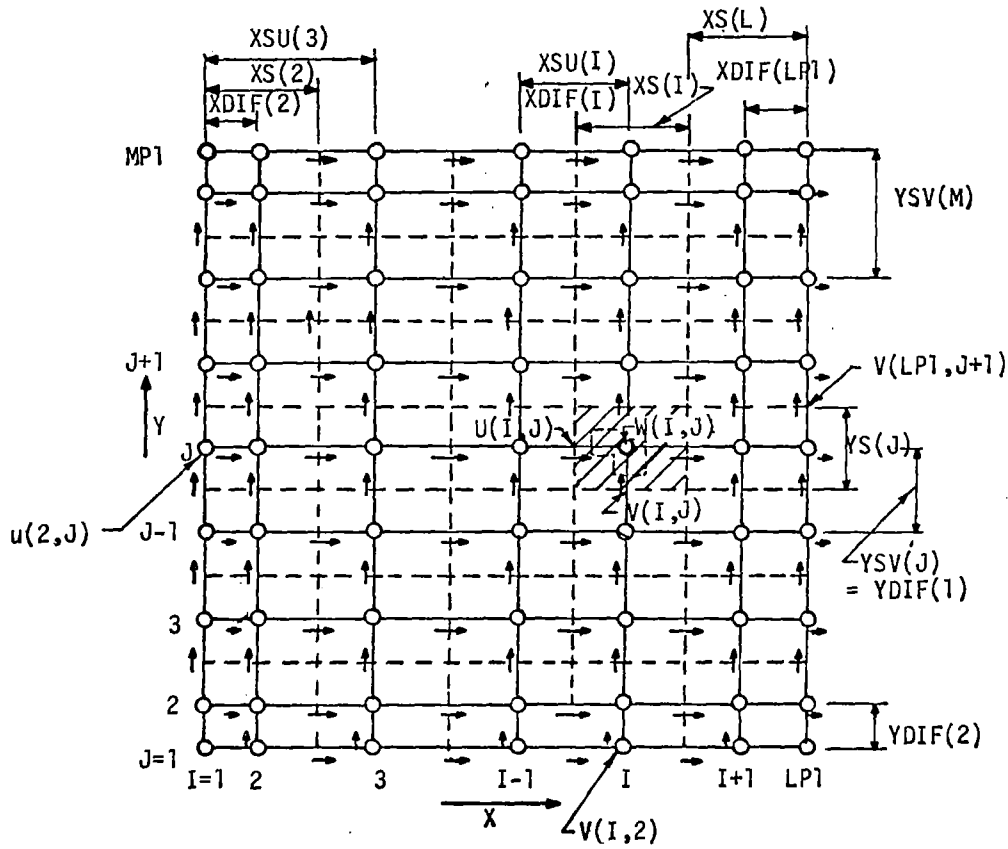


FIGURE 11: GRID SHOWING NUMBERING, MAIN CONTROL VOLUMES AND FORTRAN DEFINITION OF GRID QUANTITIES. (CARTESIAN COORDINATES)

The dashed lines in figure (11) join the control-volume faces normal to the x and y directions. These are the control volumes for all dependent variables except the u and V velocity components. The control-volume faces pass mid-way between the grid nodes except near the boundaries where they pass through the boundary grid nodes. Thus, the control-volume faces always pass through points where the velocity component normal to the faces are stored. A normal velocity component at a control-volume face is presumed to prevail over that whole face.

The control-volumes for each of the velocity components u and v are displaced along the directions of these velocities. The control-volume faces normal to each of these directions pass through grid nodes on either side of the velocity component in question. Figure (12) illustrates this point.

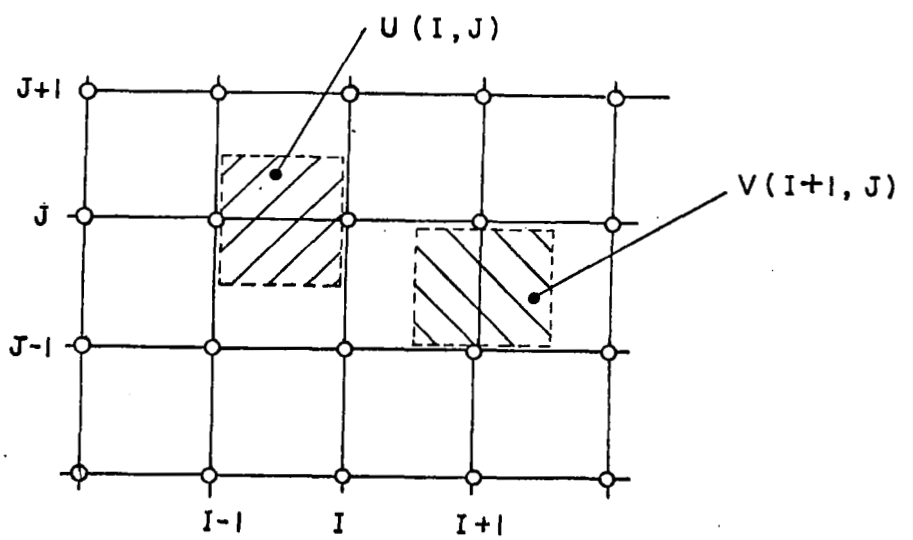


FIGURE 12: U- AND V- VELOCITY CONTROL VOLUMES

The independent variables x, y are stored as the coordinates X(I) and Y(J) of the grid lines. Certain related quantities are necessary and are calculated and stored here, either once-for-all if the domain cross-section remains unchanged, or at every station if it changes. Among these XS(I), XDIF(I) and XSU(I) are derived from the values of X(I) such that: XS(I) denotes the x-direction length of a main control-volume around the node (I,J); XSU(I) is the x-direction length of the control-volume for U(I,J). (Note that XSU(I) is the same as XDIF(I) except near the boundaries of the calculation domain). Incidentally XS(I) is also the distance between the locations of U(I,J) and U(I + 1,J) and performs the work of XDIF(I) for the equation for u. The meanings of YS(J), YDIF(J), and YSV(J) should now be obvious. The geometric quantities associated with the grid system are defined in Table 5.

Because the faces of the main control-volume are defined to pass midway between the grid nodes, interpolation factors for the calculation of variables on these faces are equal to 0.5, except near boundaries where they are either 0 or 1. For the control-volumes appropriate to U- and V- velocity components however, the interpolation factors can differ from 0.5 if the spacing between grid nodes is chosen to be non-uniform. For this reason, interpolation factors are calculated in STRID1 and stored as FXP(I), FXM(I), FYP(J) and FYM(J). The subscript refers to a grid node. The value of U for example at a grid node (I,J) is given by:

$$FXP(I) * U(I + 1,J) + FXM(I) * U(I,J) \qquad (5.2\text{-}7)$$

It is obvious from the above that FXM(I) is simply 1.0 - FXP(I). The expressions for FYP and FYM are similar.

TABLE 5. Definition of Grid Geometric Quantities

NO	GRID QUANTITY	MEANING
1	X(I)	Physical coordinate in the ξ-direction; represents x in cartesian coordinates.
2	XDIF(I)	The difference between X(I) and X(I-1); used as the distances δ in calculating ξ-direction diffusion flux of ϕ: $\Gamma_\phi \Delta\phi/\delta$.
3	XS(I)	The ξ-direction width of a main control volume.
4	XSU(I)	The ξ-direction width of a U-velocity control volume.
5	Y(J)	Physical coordinate in the η-direction; represents y in cartesian coordinates.
6	YDIF(J)	The difference between Y(J) and Y(J-1); used as the distances in calculating η-direction diffusion flux of ϕ.
7	YS(J)	The η-direction width of a main control volume.
8	YSV(J)	The η-direction width of a v-velocity control volume.

Calculation of the quantities tabulated above completes the tasks performed by STRID1. STRID1 is called once from MAIN to calculate the initial grid quantities; thereafter, if IARCH = 2, i.e. variable areas of the integration plane are to be accounted for, STRID1 is called from MAIN at every step, after a call to GEOMOD has provided the necessary information for the cross-section change.

The third section of STRIDA, namely STRID2, aids partly in the calculation of the coefficients in the finite-difference equations. STRID2 is used to calculate and store the convective mass velocities (i.e. the terms in square brackets in equation (2.3-2) crossing the control volume faces along the ξ- and η-directions.

The arrays GX and GY are used, respectively to store these values. STRID2 is called for each integration plane, once at the beginning of STRID3, then again from STRID3 after the grid has been adjusted to fit the downstream geometric configuration. Finally STRID2 is called from STRID4, after the u and v velocities have been corrected.

5.3 STRIDB

STRIDB is the largest and perhaps the most important subprogram. STRIDB is the main machinery of the SHIP program and contains instructions to calculate the 'A' coefficients in the finite-difference equations (3.2-4) and (3.2-7) to (3.2-9). The coefficients are assembled in STRIDB based on the convection and diffusion fluxes in the three coordinate directions. STRIDB contains two member subroutines: STRID3 and STRID4.

It is in STRID3, that the finite-difference equations appropriate to U, V, W and PP are assembled, in that order; while STRID4 assembles the coefficients for all other equations such as for kinetic energy of turbulence, k, etc. The first entry statement to STRIDB is STRID3. STRID3 calls first STRID2 to assemble the mass fluxes GX, GY and GZ crossing the respective cell areas. These values are computed at any section, from the upstream distributions of u, v and w.

The first equation assembled by STRID3 is the u-momentum equation. Later, in sequence, the v, w and pressure-correction equations are solved. Since the structure of FORTRAN instructions is similar for all equations, it is sufficient here to explain that for one of them only.

For the u-momentum equation, the details are as follows: The statements defining ISTR and JSTR specify the starting I value and J value for the equation. For the u-velocity equation, ISTR is 3 and JSTR is 2; for the v-velocity, ISTR = 2 and JSTR = 3; for others ISTR = JSTR = 2. The next important instruction is a call to GAMMA; GAMMA calculates the diffusion coefficients that enter the finite-difference equations. GAMMA in turn, makes a call to GAMOD whereby account is taken of the modifications for the boundaries. In the present version of SHIP, the call to GAMOD is redundant. A subsequent call to SOURCE computes the source terms in the equations. It should be noted that the SU and SP are such that:

$$S = SU + SP*\phi_P$$

where S is the source term of the equations. This source term is then integrated in STRID3 over the control volume.

The calculation of the A coefficients starts first with the calculation of the upstream convection coefficients, denoted by ALZ(IJ). These are merely the mass fluxes over the cell areas normal to the z direction. In the cross-stream the coefficients are calculated first for the near-boundary nodes.

The first statements calculate coefficients arising from the J = 1 boundary (i.e. pertaining to AYM for J = 2); and the next statements calculate those for the I = 1 boundary. Then in a DO loop, the coefficients for the other interior nodes are calculated. The AL-s represent the convection part (the L's in equation (3.2-5)), and the T-s represent the diffusion part (the hyphen stands for X or Y depending on the direction considered). The high-lateral-flux modification is then introduced. Then, the pressure gradient term is calculated; DU is the area over which the pressure forces act; and SU is the source term summed up along with the contribution of others. When all the coefficients are assembled, a call to SOMOD is made to determine whether any of the earlier computed coefficients and source terms require modification, to account for the particular flow-geometry. Once this is achieved, a call to SOLVE permits solution of the linear algebraic equations to be obtained by sweeps of TDMA.

The other subsections of STRID3 perform identical operations. First the v and w equations are solved in a manner similar to that for u. After this is done, the requirements of

overall mass continuity are examined. Then, the coefficients for the pressure-correction equation are assembled. The calculation of these coefficients is similar to that for other equations; but it is to be noted that, for the pressure-correction equation, AZ is identically zero; and the term SU is the mass source. It is important to note here that the mass flux from the downstream face (i.e. ρw^*) is calculated from an updated density at the downstream face. The pressures and velocities are subsequently corrected and this concludes STRID3.

The assembly and solution of the finite-difference equations of other dependent variables is done in STRID4. Before STRID4 is started, a call is made to STRID2; this is to calculate the new values of GX, GY based on the newly calculated u and v velocities. The operations in STRID4 are similar to those explained in STRID3.

At the end of STRIDB, the directions to perform the TDMA sweeps are given. The indices IXY, ISWP and JSWP are changed through the statements

```
IXY=2-IXY
ISWP=3-ISWP                                    (5.3-1)
JSWP=3-JSWP
```

The completion of STRID3 and STRID4 yields new distributions of all variables and the pressure $\bar{p}$ at a downstream location. The repetition of STRID3 and STRID4 at several forward steps is controlled by the main program SHIP.

5.4 Solution Procedure for Algebraic Equations

The Subprogram SOLVE

The function of the subprogram SOLVE is to arrange for the solution of the finite-difference equations, for each dependent variable NV, to be obtained. The solution procedure used is the application of a pair of TDMA traverses, one in each of the ξ-and η-directions.

SOLVE has three major sub-divisions. The first ends with the statement: 10 CONTINUE. It is in this part that the finite-difference coefficients are assembled in readiness for the subsequent operations. It is here that our fully-implicit difference scheme is implemented during the coefficient-assembly process; incorporation of other schemes will require some modification of this part of SOLVE.

The second part of SOLVE is concerned with TDMA traverses in the ξ-direction and ends with statement: 21 CONTINUE

The third and final part of SOLVE starts with this statement and concerns the TDMA traverses in the η-direction.

A call to SOLVE is made from STRID3 and STRID4, once for each dependent variable NV. This call achieves TDMA traverses in both the ξ- and η-directions; however, which traverse is made first depends upon the value of the index IXY. The first traverse direction will be ξ if IXY = 1, and η if IXY = 2. IXY is set alternately to 1 or 2 by the statement: IXY = 3 - IXY which concludes both STRID3 and STRID4.

Along each traverse direction, the direction of sweep i.e. whether from the first grid node to the last or vice versa, depends upon the value of an index, ISWP in the ξ-direction and JSWP in the η-direction. Each of these indices takes on a value 1 or 2 by statements which follow the end of parts 2 and 3 of SOLVE. For example, the statement following: 21 CONTINUE, reads JSWP = 3 - JSWP. A value 1 implies that the sweep direction is from first to last grid node and 2 implies vice versa.

On occasion, it may be required to perform more than one pair of TDMA traverses in a ξ - η plane, for any given dependent variable. The number of pairs of TDMA traverses is set by values assigned to an index array NSWP(NV). The program is set up with NSWP values equal to unity except for the pressure-correction equation for which NSWP(NPP) = 3. For locations near injection points the NSWP values are increased to ensure stability and accuracy.

5.5 Printout of Field Values of Dependent Variables

PRINT(ISKIP, JSKIP)

It is frequently required to print out the contents of the F-array. This task is performed by subroutine PRINT.

PRINT(ISKIP, JSKIP) provides for the printout of F(I,J,NV) where NV can attain a maximum value of NFPMAX, which is set as:

$$NFPMAX = NNV + 3 \qquad (5.5\text{-}1)$$

The three extra values representing NVP, NRO and NMU, i.e. pressure, density and effective viscosity respectively. The decision as to whether a particular variable NV is printed out or not, depends upon whether the corresponding IPRINT(NV) is equal to unity or not.

The printout of each dependent variable NV is given a heading stored in TITLE(...,NV). The formal parameters ISKIP and JSKIP permit the selective skipping of columns (I) and rows (J), when it is not required, for any reason, to printout the complete array of values of each variable.

6. THE PHYSICAL MODELLING SECTION OF SHIP

6.1 Introduction

This chapter describes the portion of SHIP which calculates the physical properties required in the solution procedure.

6.2 AUX

The general policy is to confine all tasks associated with physical modelling to subprogram AUX. Thus the calculation of density, ρ, effective diffusion coefficient Γ, and sources and sinks S of the dependent variables are performed in separate member subroutines in AUX, namely, DENSTY, GAMMA, SOURCE, VISCOS and SPECIE.

AUX to a large extent, is an invariant subroutine; it need not be changed unless different physical laws and turbulence model need to be incorporated. AUX is not called as such from any subroutine; instead the various parts mentioned above are referenced to when necessary.

6.2-1 DENSTY

This subroutine calculates the densities $\rho_{P,U}$ {RHO(I,J)} and ρ_P {RHOD(I,J)} in accordance with the discussion of Section 3.2-6. At each forward step new RHOD(I,J) are calculated from guessed values of pressure. After calculating the starred velocity fields, RHOD(I,J) are changed to correspond to the new velocity distribution.

6.2-2 VISCOS

The function of VISCOS is to calculate the viscosity, both laminar (if necessary) and turbulent. In its present form, the laminar contribution has been neglected, since the flows under consideration are highly turbulent. Hence, the major function of VISCOS is to store the turbulent viscosities in the array AMUT(I,J).

VISCOS also performs the function of calculating for the N,S,E and W boundaries, the effective boundary diffusion based upon the semi-logarithmic law-of-the-wall. These diffusion coefficients are stored respectively in the arrays GAMN(I), GAMS(I), GAME(J), and GAMW(J), which are later substituted in appropriate GAM locations by GAMOD.

6.2-3 GAMMA

This part of AUX is used to set values to the exchange coefficients array GAM(I,J). These are calculated simply as:

$$GAM(I,J) = AMUT(IJ)/PR(NV) \qquad (6.2\text{-}1)$$

A call to GAMOD is then made in order to permit any modifications to be made to the GAM array.

6.2-4 SOURCE

The section headed by SOURCE is concerned with the calculation of the finite-difference form of the source terms in the equations stated in Table 1. The source terms for each variable are programmed under separate subsections; and choice is made through the NV indices (e.g. NVU, NVV etc.). The source terms calculated in SOURCE are for unit volume and represent volume averages; they are multiplied in STRIDE by the volume of the appropriate control volume. The production term for the kinetic-energy of turbulence, k is calculated also in AUX, and is stored in the array GENR(IJ).

It may be noted that all source terms contain two components SU and SP. SU is that part of source terms which is calculated completely from upstream values of the variable; SP is the linearised part. In total they express combinedly the relation

$$S_\phi = SU(I,J) + SP(I,J)*F(I,J,NV) \qquad (6.2\text{-}2)$$

It is necessary to ensure that SP is always negative.

6.2-5 SPECIE

Subroutine SPECIE is used to calculate the species mass fraction from knowledge of the element mass fractions, pressure and temperature. Appendix A gives a full development of the technique employed.

7. PROBLEM-DEPENDENT SECTIONS OF SHIP

7.1 Introduction

This chapter completes the detailed description of the functions of the various portions of SHIP by discussing the subroutines which must be changed in order to specify a particular problem.

7.2 General Policy

As mentioned briefly earlier, the main machinery of the numerical calculation procedure is devoid of any problem-specification information; the latter is provided through subroutines BLOCK DATA and ALLMOD. It is envisaged therefore, that detailed modifications to the above-mentioned routines, may require to be made for each new problem and should be done so with care.

7.3 BLOCK DATA

BLOCK DATA serves to provide values to fluid properties, grid distributions, program control parameters and other information specific to each new problem, via DATA statements. The use of BLOCK DATA permits the program to be run with compilers common to both CDC and IBM machines.

In the present version of SHIP the above information is given in chapters. Thus, Chapter 1 deals with preliminary information such as SMALL, GREAT etc. Chapter 2 provides the information necessary to specify the grid and geometry. Chapter 3 is concerned with the dependent variables information and Chapter 4 with the physical properties data. Chapter 5 provides some starting values whilst Chapter 6 is concerned with step control. Chapter 7 provides the fixed boundary conditions and indices; finally Chapter 8 provides the indices required for printing-out.

7.4 ALLMOD

Subroutine ALLMOD contains instructions for incorporating specific information regarding the flow geometry, and for any specific changes to the coefficients in the finite-difference equations, or to the variables themselves. ALLMOD is divided into several "MODification" routines which will be described below. More specifically, it is composed of seven member subroutines BEGIN, GAMOD, GEOMOD, SOMOD, UPSTRM, INJMOD and INJMOT.

7.4-1 BEGIN

The primary purpose of this subroutine is to provide initial values to all the dependent variable arrays, fluid-property arrays and other auxiliary arrays, so that the marching integration can start. The inlet values of velocities, temperatures and turbulence quantities are specified here. Also here, σ_ε, the turbulent Prandtl number for dissipation of kinetic-energy of turbulence is calculated from the relation:

$$\sigma_\varepsilon = \frac{K^2}{(C_2-C_1)C_D^{\frac{1}{4}}} \qquad (7.4\text{-}1)$$

Experience with the k-ε model of turbulence has shown that the above relation, though it applies strictly to the wall region, produces satisfactory results for regions far from the wall. This relation is derived by eliminating the convection terms from the conservation equation of ε and by evaluating the production terms of ε from the logarithmic law of the wall.

The secondary purposes include provision of 'fixed' boundary conditions on the four boundaries of the calculation domain, and calculation of some auxiliary information required in the initialising process.

The preliminary calculations for incorporating the free-boundary conditions are also made here, depending on the values of the indices KBCE, KBCW, KBCN, KBCS. A free boundary is implied when the value of the above coefficients is 3.

It should be noted that the quantity MW/RT used in the above calculations for the free-stream, assumed MW = 28.93. This should change if the free-stream is not pure air. The user will be required to give careful attention to this section.

7.4-2 GAMOD

GAMOD is provided to allow the exchange coefficients GAM(I,J) computed in AUX to be modified, as necessary, to incorporate the required boundary conditions.

As a matter of fact, the contents of GAMOD in the present version of SHIP are redundant. The required modifications are made directly to the 'A' coefficients in SOMOD.

7.4-3 GEOMOD

GEOMOD is the subroutine where modifications to the geometric configuration of the calculation domain can be prescribed.

To activate GEOMOD, IARCH is set equal to two; otherwise, the geometry will be a rectangular solid set by the initial conditions. The code can handle any geometry in which there are no sudden or discontinuous changes in domain size and the cross section of the domain normal to the main flow direction is rectangular. The geometry is determined by four constants whose magnitudes are set in GEOMOD. These constants (with definition) are:

DXWDZ = rate of change of distance between reference plane and west boundary with respect to distance in the main flow direction.

DYSDZ = rate of change of distance between reference plane and south boundary with respect to distance in the main flow direction.

DBXEDZ = rate of change of width of domain with respect to distance in the main flow direction.

DBYNDZ = rate of change of height of domain with respect to distance in the main flow direction

The values of these four quantities are determined by the given domain and can either be constants or functions of distance in the main flow direction.

7.4-4 SOMOD

The purpose of SOMOD is to facilitate modifications to the source terms SU(I,J) and SP(I,J) and the coefficients in the finite-difference equations, AXM(I,J), AXP(I,J) etc. SOMOD, together with GAMOD, achieves the final form of the finite-difference equations before they are solved. At present, the function of SOMOD is to incorporate the wall functions and the symmetry boundary conditions; but a greater amount of modification, such as creating internal obstacles etc., can be achieved through SOMOD. SOMOD is divided into several sections each dealing with a separate variable. For the equation for pressure-corrections no modifications are made.

As mentioned earlier, the provision of wall-functions is made through SOMOD. This is achieved as follows: first, coefficients linking boundary grid nodes with their immediate neighbours inside the calculation domain are set to zero for each variable. This is done because, by incorporating the wall functions, we are prescribing the values of the fluxes directly; and hence whatever values are calculated earlier in STRIDE for the coefficients must be set to zero. Then if an index, for example, KBCS for the South boundary, is set equal to unity, the appropriate wall flux is calculated and fed in through SU and SP. This calculation uses the value

of GAMS(I) (calculated in AUX, and brought here through a COMMON statement); and the corresponding flux, FLUXS(I,NV) of the dependent variable is stored for purposes of print-out. If the index is other than unity, no change is made to the coefficients. Similar indices KBCN, KBCE and KBCW are used for the North, East and West walls. Note that for the v-velocity, for example, there are no modifications for the North and South walls since they are normal to that velocity. For the w-velocity the wall functions for the above wall boundaries are similar to that for u. Such checks and modifications are made for the variables u, v, w, k, ε, h and f.

The modifications to the source term for k consist of altering the generation and dissipation based on shear-stress from the wall functions. For the dissipation equation, the value of dissipation is fixed according to equation (3.4-4), by modifying SU and SP. Setting SP to a large negative value (-10^{30}) and SU to a large positive value multiplied by the required value to be fixed ($10^{30}\varepsilon_{fix}$), we nullify the effect of other coefficients (since they will be divided by SP), and obtain ε equal to the desired value ε_{fix}. This practice is adopted in general for fixing any variable at a desired value.

The user of course may be required to provide other types of boundary conditions himself, again through SU and SP. In this respect, choices of the index values other than unity can be profitably put to use.

7.4-5 UPSTRM

The subroutine UPSTRM makes provision to store upstream (i.e. previous integration plane) values of pressure which are necessary in calculating the source term of the axial velocity component. The upstream values of the width and height of the integration domain are also stored here, for variable geometrical configurations. UPSTRM is also a convenient place to calculate the axial direction mass flow rate. It should be noted that upstream values of any other variables apart from pressure are not required to be stored. This should be the case only if iterations were necessary.

7.4-6 INJMOD

This subroutine is primarily used to specify the correct flux of a given variable through the array FINJ(NV). This array is used to modify the source term in SOMOD when injection occurs through the South wall.

7.4-7 INJMOT

This subroutine has a function identical to that of INJMOD above, but for injection occuring through the North wall. INJMOT and INJMOD may be called either simultaneously or separately from MAIN; this depends on whether injection occurs through both walls or through either wall and is also decided in MAIN.

8. SOME USER'S GUIDANCE IN ADAPTING SHIP FOR A GIVEN PROBLEM

8.1 General Remarks

The following steps are necessary in adapting SHIP for a given problem.

a. Provide the following information in BLOCK DATA

- Program control parameters
- Grid and geometric specifications
- Printout control parameters
- Solution procedure parameters
- Fluid property values
- Thermodynamic and hydrodynamic data appropriate to the problem
- Fine-tuning of the turbulence model constants to optimise the results.

b. Provide adequate initial values to variables in BEGIN. It may be required, for example, to chose a grid disposition (ZETA (I) and ETA (J)) to suit known initial distributions of dependent variables.

c. Check if known boundary conditions are correctly set and unknown values correctly calculated.

d. Incorporate the exact geometric configurations of the problem into the appropriate sections of ALLMOD.

e. Arrange in PRINT, for requisite printout

8.2 List of Input Variables

Following is a list of input variables to be supplied to the SHIP program; they correspond to the variables defined in the BLOCK DATA routine at the beginning of the program. The following information is given for each variable.

(i) the FORTRAN symbol

(ii) the meaning

(iii) for some variables, the recommended value is given in the last column.

SYMBOL	MEANING	REC VALUE
	1. For Program Control	
IMAX JMAX	They correspond to the dimensions of the major arrays.	
NNV	The number of variables (NV) for which the F array is dimensioned.	
NPP, NVU, etc.	They are variable numbers having values ranging from 1 to 10.	
ISTEP	The step number; it is initialised in BLOCK DATA.	0
IARCH	Specifies whether the flow is to be treated as: one of constant geometry, or varying with axial direction.	 1 2
FRA	The initial step length.	
FRAM	The maximum step length.	
EX	Expansion factor for step length. FRA at step n, (FRA_n), is equal to FRA_{n-1}*EX or FRAM whichever is smaller.	
SMALL, GREAT	Small and large numbers used at various places in the program.	10^{-30} 10^{30}
	2. Grid and Geometry Variables	
LCV	Total number of control volumes in the ξ direction.	
MCV	Total number of control volumes in the η direction.	
ZETA	The disposition of grid nodes in the ξ direction. ZETA ranges from 0 to 1 always and is given, in general, by $\text{ZETA(I)} = \frac{\text{X(I)}}{\text{BXE}}$.	
ETA	The locations of the grid nodes in η direction $\text{ETA(J)} = \frac{\text{Y(J)}}{\text{BYN}}$.	

SYMBOL	MEANING	REC VALUE
KBCN KBCS KBCE KBCW	Specify the nature of the North, South, East and West Boundaries. Thus for: Wall boundary Symmetry axis Free boundary	 1 2 3
BYN	Height of the domain. BYN must be initialised to the value at the inlet plane.	
BXE	The extent of solution domain in the x-direction.	
ZU, ZD	Axial locations of upstream and downstream computational planes - must be initialised here.	0.0
DZ	Axial step length. The value set here is overwritten by that calculated from FRA specification.	
DYSDZ	dy_S/dz - initialised here to zero.	0.0
DBYNDZ	d(BYN)/dz - initialised here to zero.	0.0
ZLAST	The z location at which solution is terminated.	
	3. Control Variables for Printout	
ZRE	The 'z' locations of the axial stations at which the distributions of the variables are printed out.	
LASTEP	The total number of axial steps at which the variables are to be calculated. At present it should be set to a large value so that the solution is terminated by ZLAST.	
NPJUMP	The number of steps between successive printouts of the variables.	
ICJUMP	Has the same meaning as NPJUMP; but it controls printout of wall fluxes.	
IPRINT (NV)	Specifies whether the distribution of the NV variable should be: Printed Not printed	 1 0

SYMBOL	MEANING	REC VALUE
	4. Solution Procedure Parameters	
ISOLVE (NV)	The value of ISOLVE(NV), specifies whether or not variable number NV is to be solved for. ISOLVE = 0 does not solve for the variable ISOLVE = 1 solves for the variable.	
NSWP (NV)	Number of TDMA sweeps performed on variable NV at each step.	6 for NV=1 and 3 for all others
IXY ISWP JSWP	These variables control the order of TDMA sweeps at each step. Recommended starting values are unity for all.	1,1,1.
	5. Turbulence-model Constants	
C1		1.44
C2		1.92
CD		0.09
AK	K in the log law.	0.42
EE	E in the log law.	9.00
PR(NV)	Turbulent Prandtl numbers for the variables. Their values are set initially to unity. However for the dissipation of ε, PR is later calculated from the expression PR(NV) = $K^2/((C_2-C_1)\ C_D^{\frac{1}{4}})$; further, PR for enthalpy is somewhat less than unity, equal approximately to 0.90.	
AKFAC	Factor relating turbulence energy to mean motion energy.	0.004
PJAY	The P function in the "wall functions" (resistance of laminar sublayer).	
	6. Fluid Properties	
PRLAM (NV)	Laminar Prandtl number for variable NV	

SYMBOL	MEANING	REC VALUE
WM GASCON	Molecular weight and universal gas constant for the gases considered. At present GASCON is taken to be 8314 $m^2/sec^2{}^oK$	
AMUREF	Reference laminar viscosity.	
DEN	Reference density.	
CP	Specific heat.	
CPDCV	Specific heat at constant pressure divided by specific heat at constant volume.	1.4
HO	Enthalpy of formation.	
	7. Starting Values	
UIN VIN WIN	Inlet x-, y- and z- direction velocities.	
PIN	Inlet pressure.	
TIN	Inlet free stream temperature.	
RETRAN	Transition Reynolds number.	
	8. Boundary Conditions	
IINJ IINJT	Indices to control entry to INJMOD and INJMOT, respectively.	
INJSTP INJTOP	Values of ISTEP at injection locations on the South and North walls, respectively.	
ZINJ ZINJT	z locations of injection, for the South and North walls, respectively.	
TINJ TINJT	Jet temperatures, for the South and North walls, respectively.	
FLOINJ FLOINT	Mass flow rates injected by a jet through the South and North walls, respectively.	
IADIAN IADIAS IADIAW IADIAE	Indices specifying whether the North, South, West and East walls, respectively are adiabatic (=1) or under constant temperature (=0).	

SYMBOL	MEANING	REC VALUE
TWALLN TWALLS TWALLW TWALLE	North, South, West and East wall temperature, respectively.	

The units used by the program are: Kg, m, sec. It may be convenient, however, for a number of input quantities to be specified in other units; this can be done provided that the conversion to Kg, m, sec is then effected internally.

A complete list of FORTRAN variables is given in Appendix C.

8.3 The Grid

- The axial grid is specified via the variables FRA, FRAM and EX, defined in the list above.
- To change the grid distribution in x and y, while retaining the same total number of nodes in each direction, simply reset the ZETA (I) and ETA (J) arrays.
- If the number of grid nodes is to be changed, then LCV and MCV must be reset, and ZETA and ETA must be respecified. Note that the number of ZETA values provided must be LCV + 2, and the number of ETA values must be MCV + 2.
- When the number of grid nodes is increased it may be necessary to redimension some of the arrays, as it is described below.
- Note that, whenever the grid distribution is changed, it will be necessary to reset the inlet conditions accordingly.

8.4 Dimension Changes

The quantities IMAX, JMAX and NNV must be set to correspond to the required dimensions of the arrays in I, J and NV (thus IMAX $\geq$ LCV + 2, and JMAX $\geq$ MCV + 2). The arrays must then be dimensioned as given in the table below, and the EQUIVALENCE statement must be modified to read:
EQUIVALENCE (F(1),PP(1)), (F(IMAX*JMAX + 1), U(1)), (F(2*IMAX*JMAX + 1), V(1)), (F(3*IMAX*JMAX + 1), W(1)), (F(4*IMAX*JMAX + 1), AKE(1)), (F(5*IMAX*JMAX + 1), ADS(1)).

Array	Must be dimensioned
1. General	
F	(IMAX*JMAX*NNV)
P, RHO, GAM, SU, SP, DU DV, DW, AXP, AXM, AYP, AYM, AZ, GX, GY, GZ	(IMAX*JMAX)
CY	At least (LCV + 2)
A, B	At least the greater of (LCV + 2) and (MCV + 2)
CYU	At least (LCV + 2)
DRHODP, PU, RHOD	(IMAX*JMAX)
PP, U, V, W, AKE, ADS	(IMAX*JMAX)
NFM	At least (NNV + 7)
ZETA, X, XS, XDIF, XSU	At least (LCV + 2)
YSR, ETA, Y, YS, YDIF, YSV	At least (MCV + 2)
FXP, FXM	At least (LCV + 2)
FYP, FYM	At least (MCV + 2)
JM	At least (MCV + 2)
ISOLVE	At least (NNV)
RELAX	At least (NNV + 3)
NSWP	At least (NNV)
IPRINT	At least (NNV + 7)
TITLE	(6, at least NNV + 7)
ZRE	At least (no. of printout stations required)
AMUT, CPMN	At least (IMAX*JMAX)
PRLAM, PR	At least (NNV)
FLUXN, FLUXS	At least (LCV + 2,NNV)
FLUXW, FLUXE	At least (MCV + 2,NNV)

Array	Must be dimensioned
GAMS, GAMN	At least (LCV + 2)
GAME, GAMW	At least (MCV + 2)
2. Subroutine PRINT	
X1	At least (LCV + 2)
X2	At least (MCV + 2)
3. Subroutine AUX	
DUIDXJ	(3,3)
GENR	At least (LCV + 2, MCV + 2)
4. Subroutine ALLMOD	
FINJ, FINJT	At least LCV

8.5 Interpretation of Output

(a) Preliminary output

This is provided by the program before the marching integration commences. It comprises the conditions at inlet, printed out as described below.

The variables printed are as follows:*

- the x-direction velocity component (m/sec)
- the y-direction velocity component (m/sec)
- the z-direction velocity component (m/sec)
- the turbulent kinetic energy (m^2/sec^2)
- the dissipation rate of turbulence energy (m^2/sec^3)
- the stagnation enthalpy (Kcal/Kg)
- the hydrogen mass fraction in any form
- the thermodynamic temperature (^oK)
- the static pressure (N/m^2)

*Note that the user is free to suppress printout of any of these variables by use of the IPRINT array.

- the density (Kg/m^3)
- the diffusion coefficient for F(Kg/m sec)
- the mass fraction of H_2
- the mass fraction of O_2
- the mass fraction of OH
- the mass fraction of H_2O
- the mass fraction of H
- the mass fraction of O
- the mass fraction of N_2
- the mass sources in the field

The printout is of the same format in each case. First is printed the heading (i.e. TITLE (6,NV)) for the variable in question. Then the complete two dimensional field is printed, with I arranged horizontally, and J vertically. Also shown are, at the far right hand side, the Y-direction grid locations for each J, normalised by the height of the domain, and below the array, the X-direction grid locations for each I, in (m).

(b) Main Output

The output provided during the marching integration is of four kinds, as follows:

(i) At every step, a single line of information is printed out. Variables are provided, which have the following meanings:

ISTEP - step number

ENTRN - the entrainment in the Y-direction through the North boundary

TOTM - the total mass flux in the axial direction

TOTW - the total momentum flux in the axial direction

TOTH - the total convective enthalpy flux

TOTN2 - the total convective flux of Nitrogen

TOTF - the total convective flux of Hydrogen in any form

FLOBOT - the jet mass flux through the South wall

FTOP - the total Hydrogen in any form mass flux at the North boundary

The headings provided for the above variables are: ISTEP, E, M, MO, H, N2, F, B and BT respectively.

(ii) At every step another single line of information is printed out. Variables are provided which have the following meanings:

ISTEP - step number

ZU - axial location, z (m)

Y(MP1) - the location of the north boundary (useful in checking the axial variation of the domain's height).

SUM - the sum of mass sources, indicating the imbalances in the field.

The headings provided for the above variables are: ISTEP, ZU, DEL and MASS IMBALANCE.

(iii) Every ICJUMP steps, axially directed wall shear stresses are printed out; drag coefficients and Stanton numbers are also printed out. What is printed out is, for I from 2 to LCV + 1.

- AREAS, AREAN, AREAW and AREAE - the areas (in m^2) of the South, North, West and East walls adjoining the near-wall control volumes for the I in question
- TAUS, TAUN, TAUW and TAUE - the local wall shear stresses at the South, North, West and East walls.
- CFS, CFN, CFW and CFE - the local wall shear stresses at the South, North, West and East walls, divided by the mean dynamic head ($\frac{1}{2}\rho w^2$) at the station under consideration
- STANS, STANN, STANW, and STANE - the Stanton numbers at the South, North, West and East walls

Apart from the above local quantities, are also

printed out mean quantities as follows:

- WBAR - the mean value of w across each plane of calculation
- DHEDTD - the mean dynamic head at each plane of calculation
- CFSAV, CFNAV, CFWAV, CFEAV - the mean values of CFS, CFN CFW and CFE defined above, respectively.
- STASAV, STANAV, STAWAV, STAEAV - the mean values of STANS, STANN, STANW and STANE defined above, respectively.

It is also in this context that the following quantities are printed out for testing purposes:

- FLOWT - the mass flow rate across each plane of calculation
- DHED - the total momentum across each plane of calculation.

(iv) Every NPJUMP steps, and/or as specified via ZRE, complete variable printout is provided as described in Section 8.5 (a) above.

9. RESULTS AND DISCUSSION

9.1 Introduction

Sample results for three typical cases of interest are presented in this chapter. It should be noted that only the third case is the novelty of this section which has, otherwise, been taken from a previous report {6} of the HISS program. This case concerns parallel hydrogen injection in a domain whose North boundary wall expands with axial distance. The results for the other two cases have been taken from {6} and have been obtained by using HISS rather than SHIP. However, test runs for identical cases, using the latter program proved that the results thus obtained are very similar to the ones reported here.

9.2 Presentation of Typical Results

9.2-1 Introduction

Results for ten cases were calculated for the contract {6} by the technique described in the first eight chapters. For each case profiles of 19 variables described earlier were computed for a grid of 12 grid lines transverse to the flow and 20 grid lines normal to the flow for a total of 240 points at each station in the main flow direction. Computations were made for several hundred stations. Thus, the total number of variables computed approaches nearly one-million for each case. In this section results for two typical cases will be presented. These results consist of hydrogen concentration, temperature and pressure distributions at three axial locations and at two locations transverse to the main flow direction.

9.2-2 Definition of cases

One case for normal injection (Case 1) and two cases for parallel injection (Cases 9 and 7) are described in this chapter. The geometrical configuration of these cases are shown in Figures 1, 2 and 3 respectively. Table 6 defines the flow and thermal properties.

TABLE 6: DEFINITION OF PROPERTIES

Location	Property (units)	Case 1	Case 9	Case 7
Main Stream conditions	Flow speed (m/s)	675	1585.2	1585.2
	Temperature (^{o}K)	70.6	1178.6	1178.6
	Mass fraction N_2	.7676	.487	0.487
	Mass fraction 0_2	.2325	.263	0.263
	Mass fraction H_20	0.0	.25	0.250
	Pressure (N/m^2)	8720.0	179300.0	179300.0
Jet conditions	Flow speed (m/s)	1210.0	2039.4	2039.4
	Temperature (^{o}K)	250.0	150.3	150.3
	Mass fraction H_2	1.0	1.0	1.0
	Pressure N/m^2	212000.0	179300.0	179300.0
	Mass flow Kg/sec	.000165	.0109	0.0109
Boundary		Ducted*	Free	Ducted*

*Duct dimensions are .0381 x .177 meters

9.3 Graphs of Results

All data are presented for planes normal to the wall and parallel with the main flow direction. One of these planes is located in the transverse direction directly at the hydrogen jet centerline and the other is located between jets (see Figures 1 and 2). The comparison of profiles at a given plane at various main flow stations indicates the rate of movement of hydrogen in a direction normal to the flow.

Figures 13 through15 are for normal injection (Case 1). Figure 13 shows the distribution of hydrogen in any form at three axial locations (.118m, .216m and .246m). The first profile is before the injection point (.186m) and therefore no hydrogen is present. At the .216m location, the hydrogen concentration levels (less than .01) indicate that substantial mixing is primarily in the y direction. (The close spacing of the adjacent injectors limits x direction mixing). Examination of the results at the .246m station shows continuing movement of hydrogen upward with an attendant smoothing of the profile, as would be expected.

The temperature profiles of Figure 14 indicate that after injection and combustion that little transverse thermal gradient exists. This is partly due to the fact that the flame front is at the outer layer of the hydrogen zone which tends to diffuse the temperature in the transverse direction. Also it is seen that the reaction of hydrogen moves the thermal boundary layer outward from the plate with movement in the main flow direction.

The pressure distribution for Case 1 is shown in Figure 15 It exhibits the qualitative behaviour one would expect. There is little transverse pressure difference due to low velocities in that direction. A pressure spike can be seen downstream of the jet indicating a shock. The pressure below the shock is essentially uniform at a higher value than the free stream. It must be emphasized that the pressure distribution in the jet region is subject to error due to the fact that the flow was forced to be parabolic when in actuality there is some upstream effect caused by the jet.

Figures 16 through 18 are results for Case 9 which is parallel injection. The diameter of the jets and jet spacing are much larger than for Case 1. The profiles at injection (z=0) show that there is little mixing of hydrogen between jets. However, as the flow moves forward

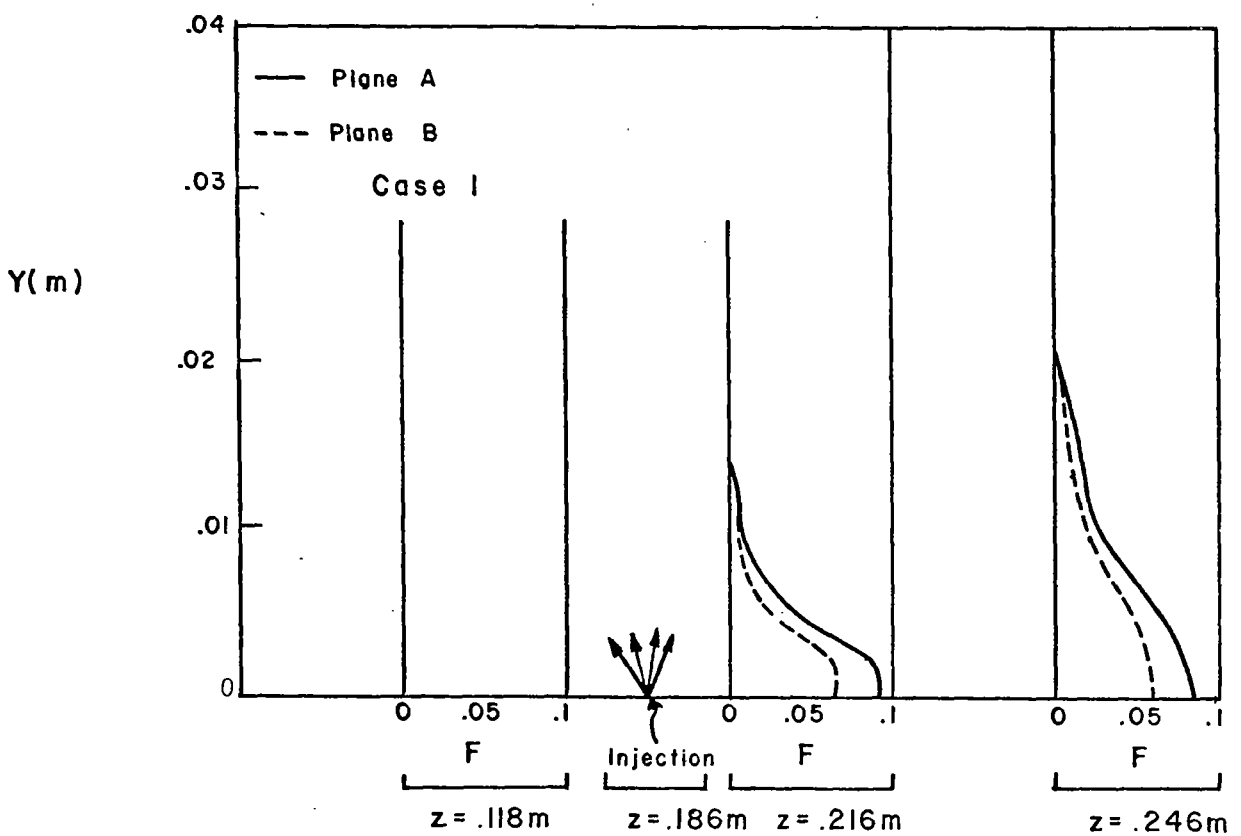


FIGURE 13: DISTRIBUTION OF HYDROGEN IN ANY FORM FOR CASE 1

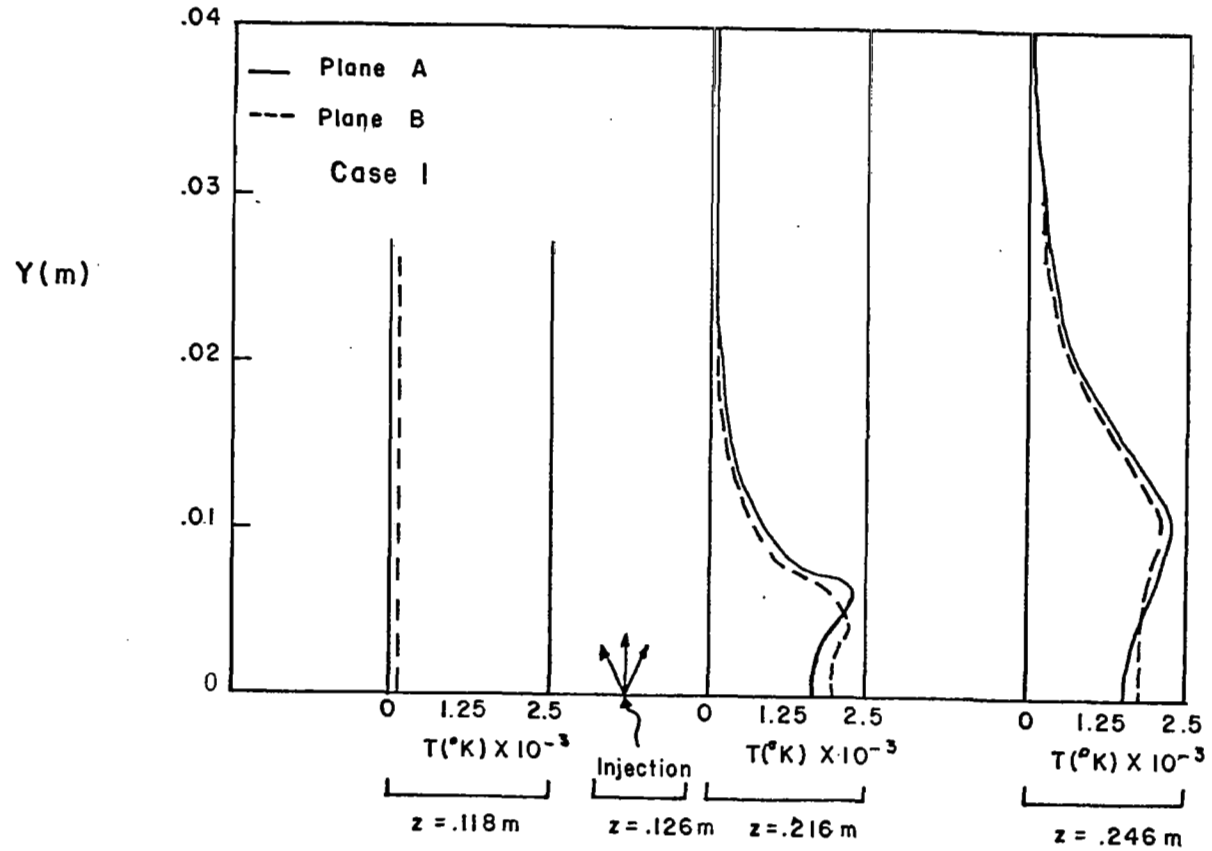


FIGURE 14: TEMPERATURE DISTRIBUTION FOR CASE 1

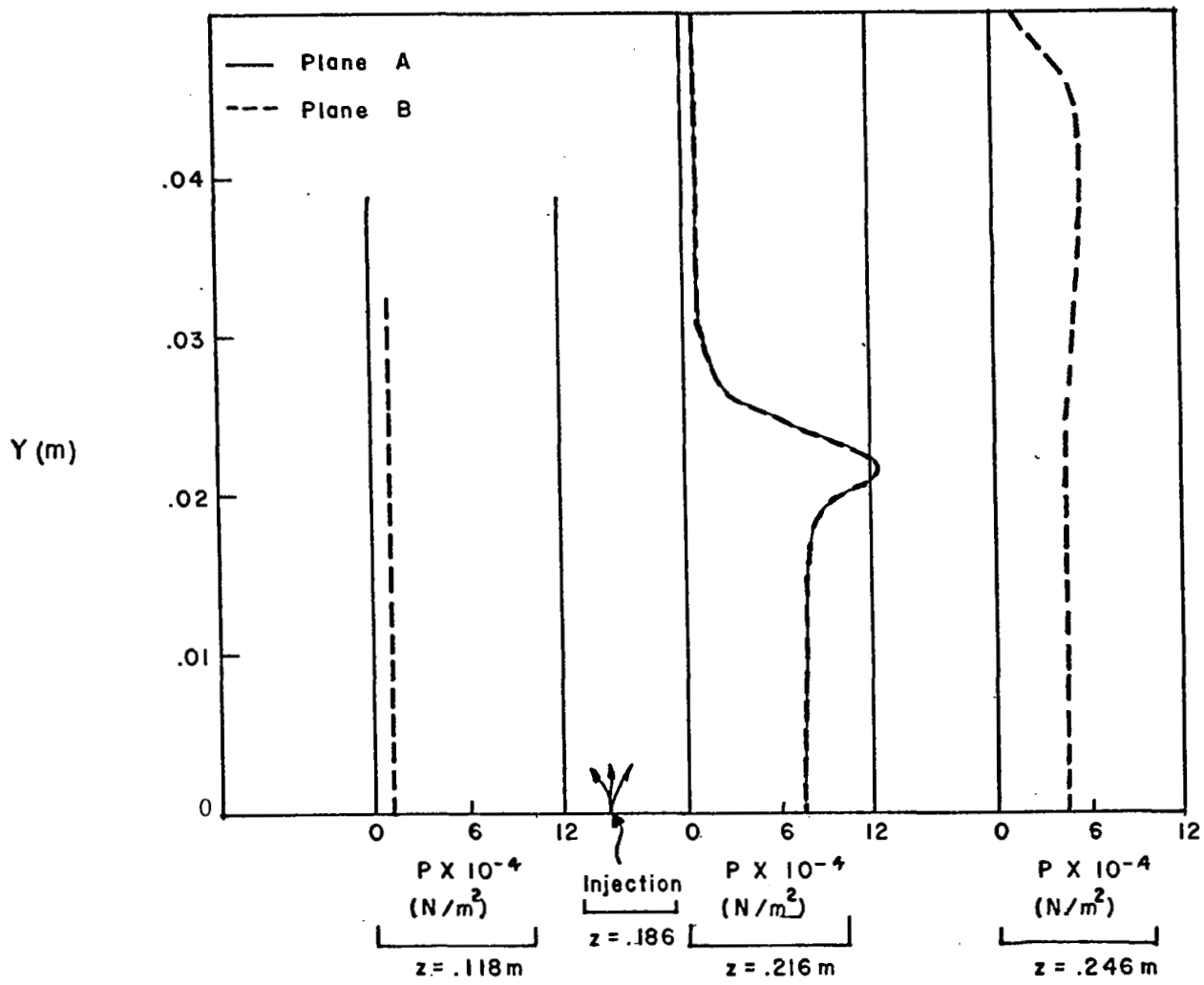


FIGURE 15: PRESSURE DISTRIBUTION FOR CASE 1

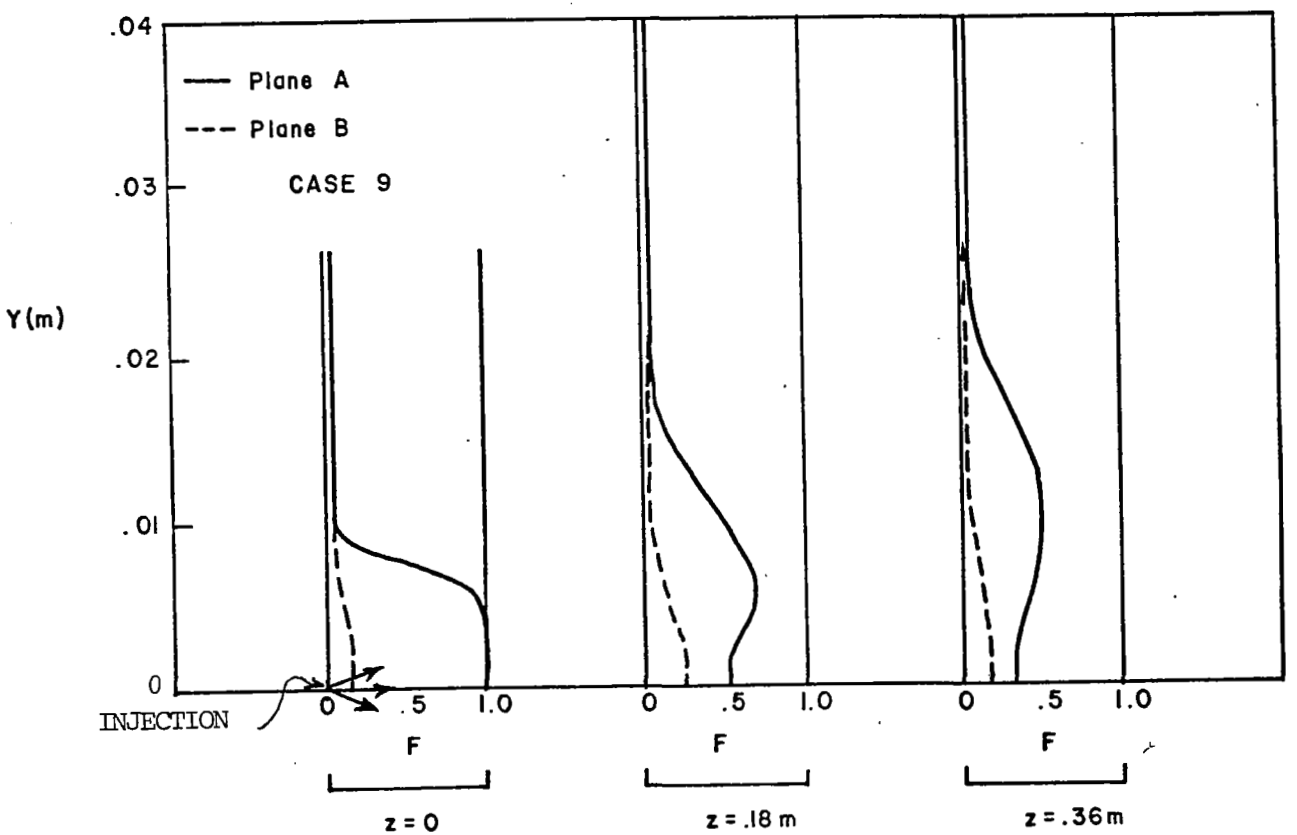


FIGURE 16: CONCENTRATION OF HYDROGEN IN ANY FORM FOR CASE 9

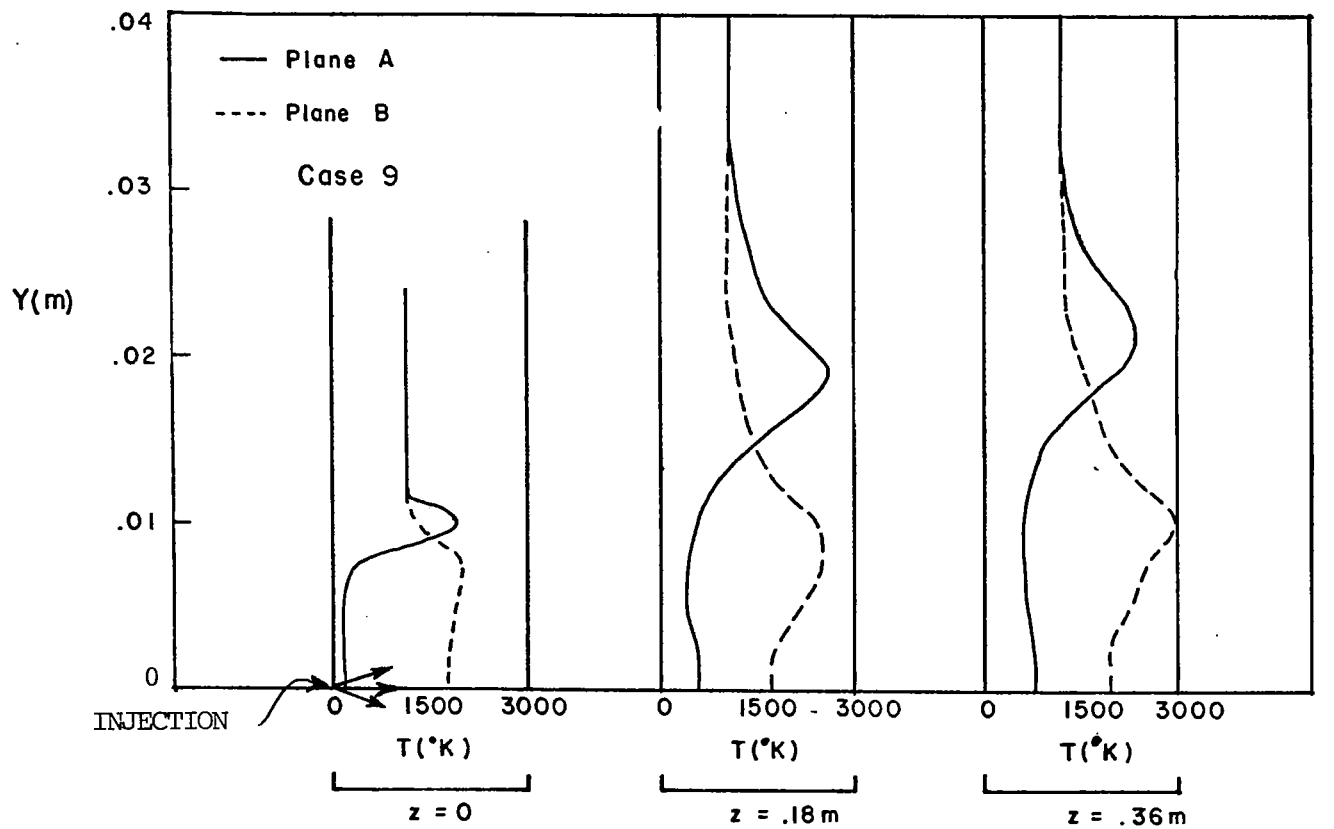


FIGURE 17: TEMPERATURE DISTRIBUTION FOR CASE 9

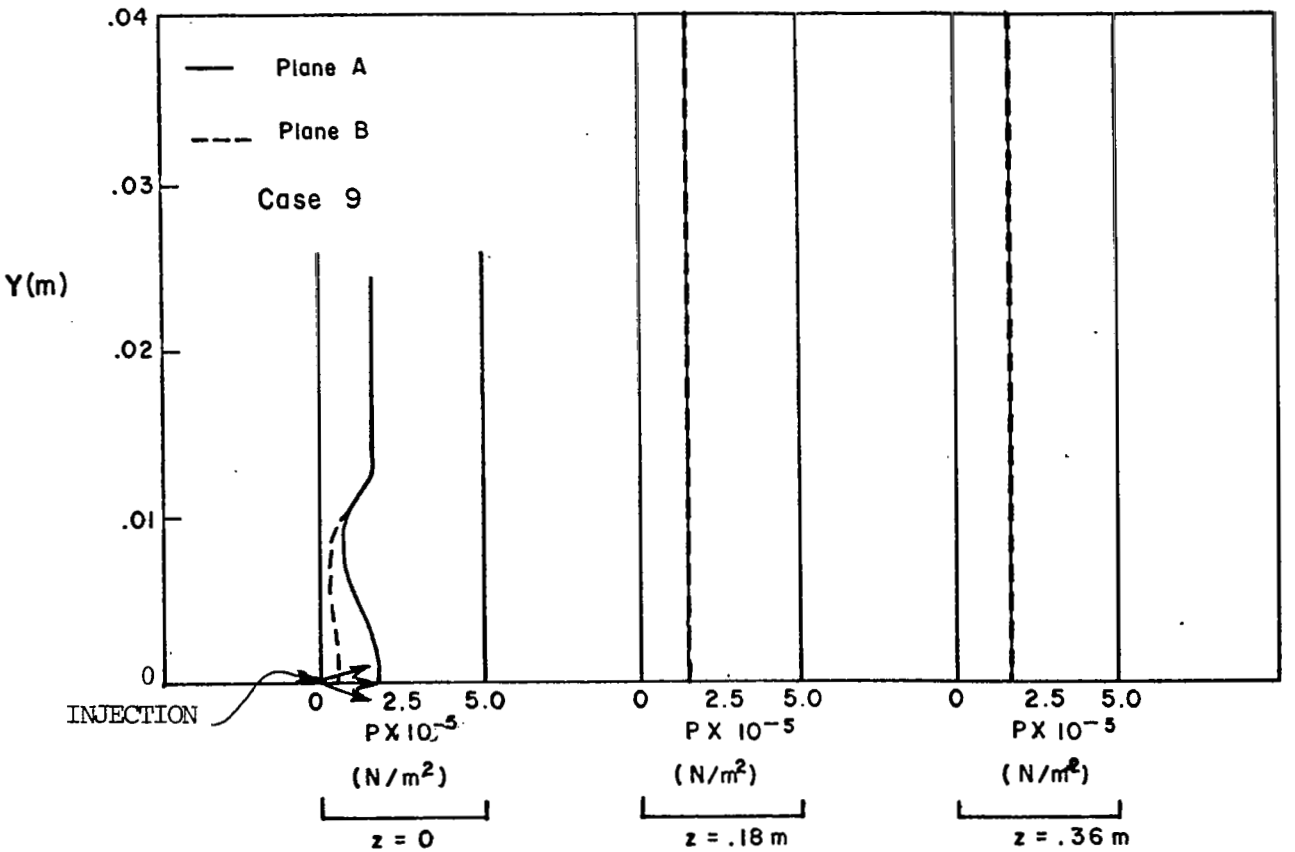


FIGURE 18: PRESSURE DISTRIBUTION FOR CASE 9

the mixing increases such that the concentration of hydrogen between jets is roughly 50% of the hydrogen concentration in line with the jet at z=.36 meter. However, these figures show that in the normal direction the movement of hydrogen upward between jets is not very effective. This is due to the low normal velocities for the parallel injection case. The temperature distribution in Figure 17 indicates a higher temperature between jets even though the hydrogen concentration is lower. This is because the combustion occurs at the fringe of the hydrogen zone. The combustion zone upper surface is indicated by the "spikes" in the temperature profile. This combustion is seen to grow with movement downstream. The pressure distribution shown in Figure 18 does not indicate any shocks. At the injection station (z=0), the flow expands in the low density region. However, at downstream locations the pressure becomes uniform at approximately the free stream value.

9.3-I Parallel injection into a duct with expanding top wall

This is the case chosen to demonstrate the validity of the SHIP program.

Profiles of 19 variables described earlier were computed for a grid of 12 grid lines transverse to the flow and 12 grid lines normal to the flow for a total of 144 points at each station in the main flow direction. Computations were made up to z=0.50m (see Figure 3) for 150 stations. In this section the results thus achieved will be presented. They consist again of hydrogen concentration, temperature and pressure distribution at four axial locations and at two locations transverse to the main flow direction. (Figures 19, 20 and 21).

The concentration profiles at injection (z=0) (Figure 19) show again that there is little mixing of hydrogen between jets. Downstream the same arguments as for Case 9 above still hold true. The temperature distribution in Figure 20 indicates again a higher temperature between jets even though the hydrogen concentration is lower. The pressure distribution (Figure 21) does not indicate any shocks. At the injection station (z=0), the flow expands in the low density region. At downstream locations the pressure becomes uniform at approximately the free stream value up to the point where expansion of the domain starts. Downstream that point the pressure is again uniform, but at lower values as we proceed further downstream.

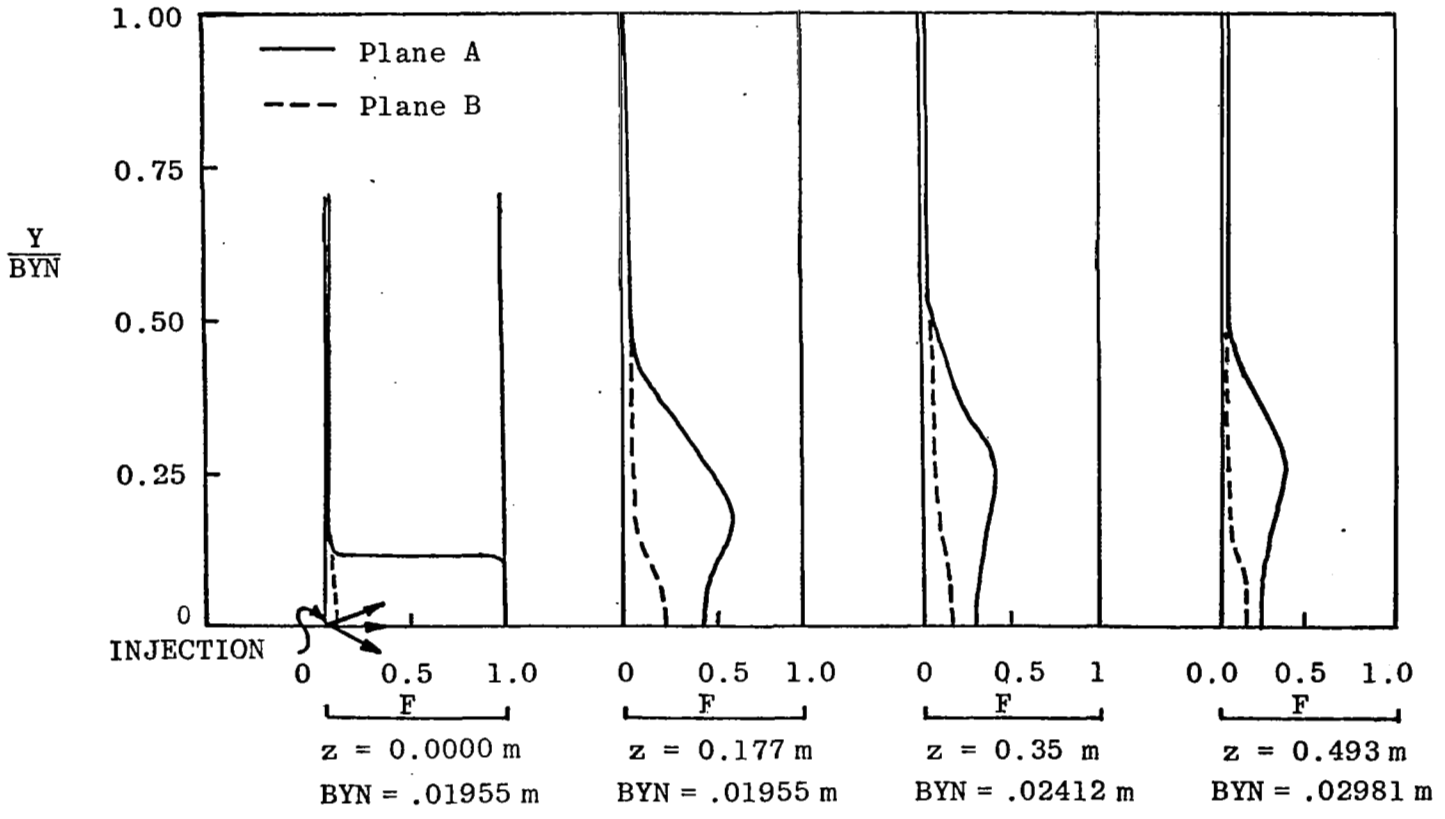


FIGURE 19: CONCENTRATION OF HYDROGEN IN ANY FORM FOR CASE 7

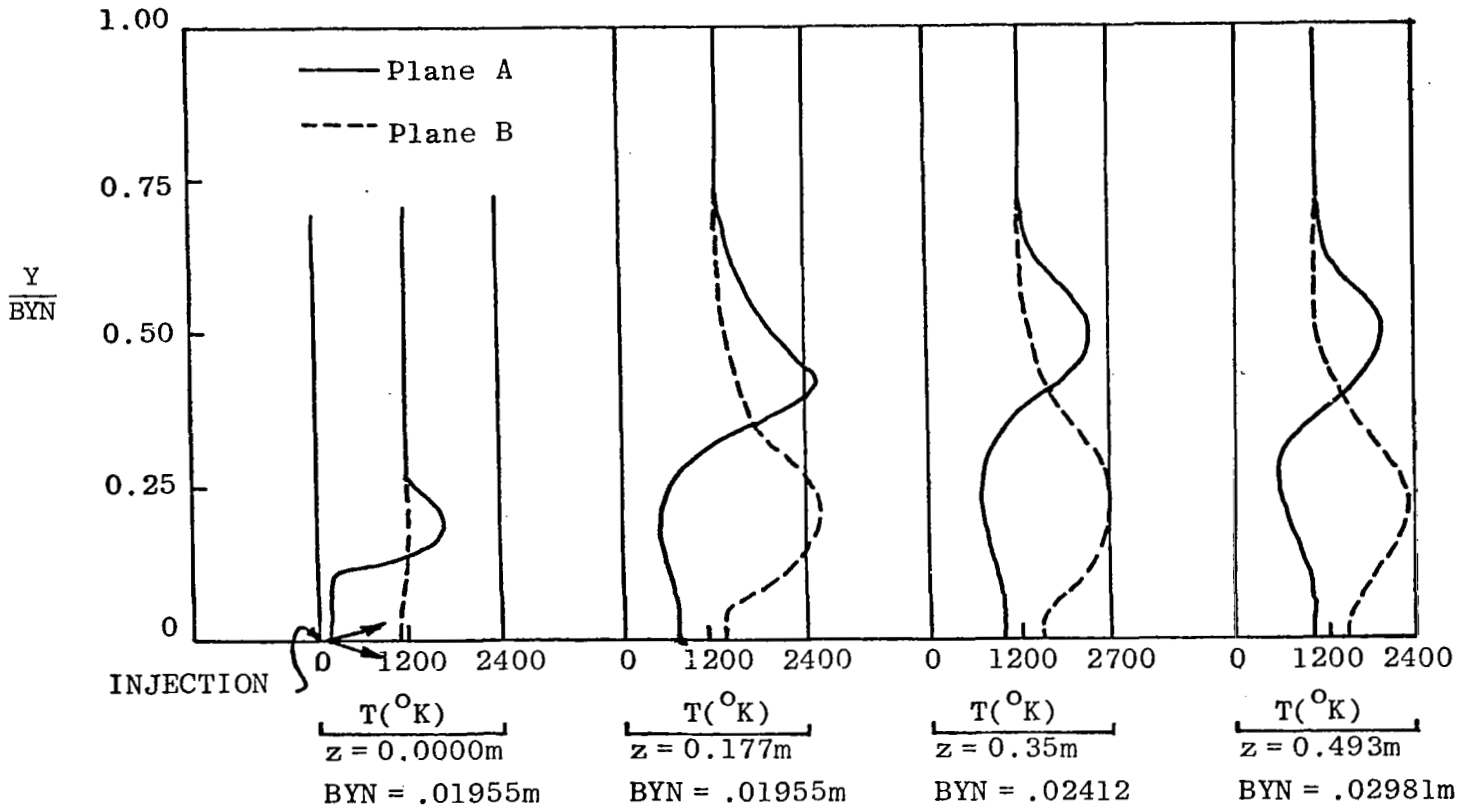


Figure 20: TEMPERATURE DISTRIBUTION FOR CASE 7

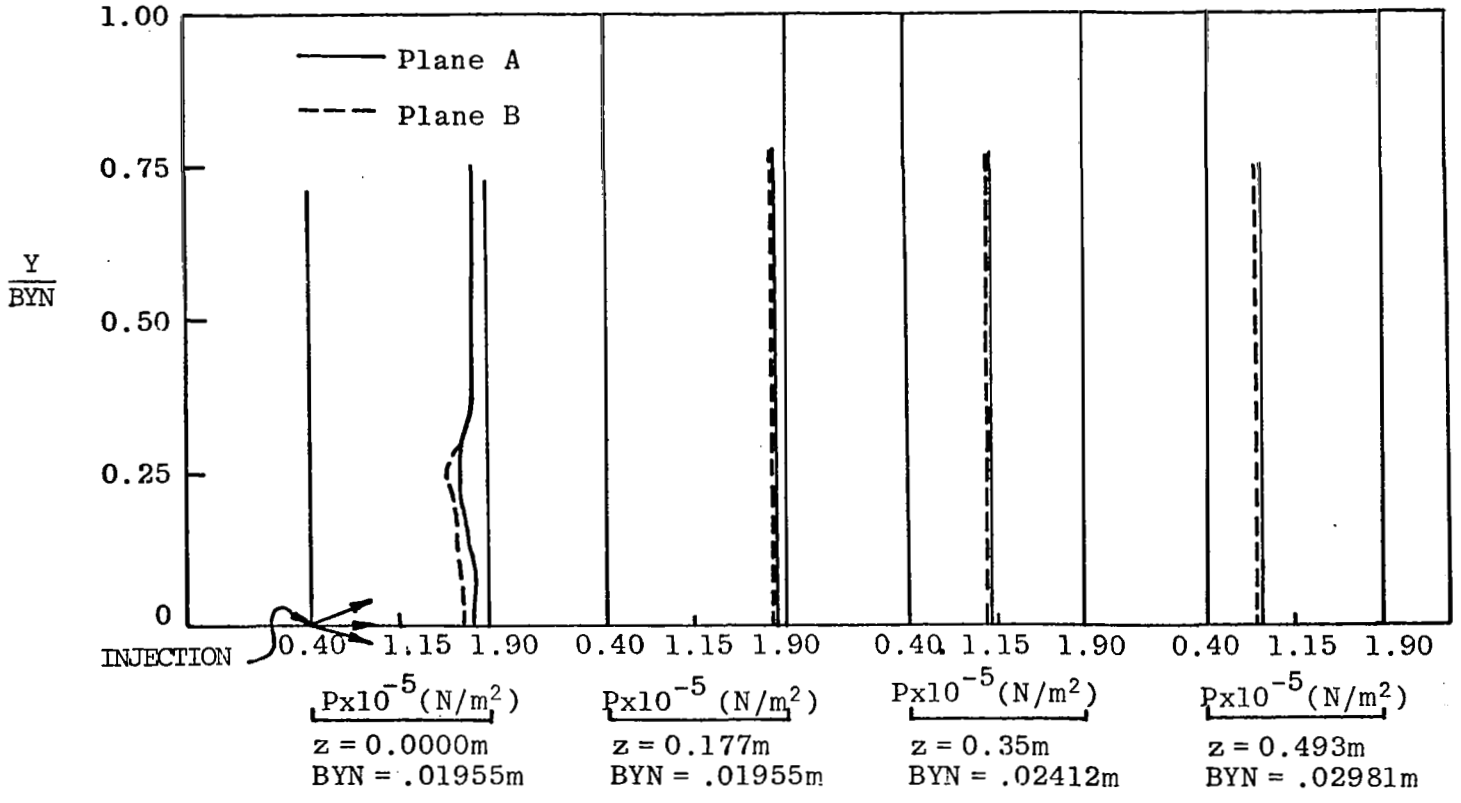


Figure 21: PRESSURE DISTRIBUTION FOR CASE 7

10. CONCLUSIONS AND RECOMMENDATIONS

Qualitatively the results obtained by the method developed herein appear to be correct. Further, comparison with cold flow data also show excellent agreement. The computational time for these results is also very good.

The assumption of parabolic flow in the injection region needs improvement because both data and calculations made in this work indicate that the pressure distribution is affected upstream by the jet. Recirculation, however, is probably not important. What is needed is a technique to allow the pressure to be calculated via an elliptic procedure and the velocity by a parabolic one. Such a technique is advantageous over fully elliptic procedure because storage and computation time are much lower.

The SHIP code has considerable potential for further development and exploitation. The suggestions made here are by no means exhaustive, but are merely intended to be pointers. Two distinct (but related) possibilities exist.

Firstly, the code can be extended to handle other, more complicated situations by suitable modifications. Secondly, it can be varied to produce new codes capable of solving new problems. At the present time the following suggestions seem worth recording. More improvements may be introduced into the SHIP code to increase its efficiency. As a matter of fact a number of latest advances are now available and may be transferred to the SHIP code. They include major reprogramming for improving the numerical algorithm (e.g. use of a different differencing scheme) and making the code more readily understandable.

A disadvantage of the present version of the code is that both velocities and pressures are stored at the same axial position (i.e. they are not staggered in the predominant flow direction). Staggering the velocity locations even in that direction and using different density interpolation formulae, will have several advantages; apart from others this practice has also the distinct merit that it blends smoothly with the elliptic and partially-parabolic ones.

APPENDICES

APPENDIX A

The Chemical Equilibrium Model

The main features of the equilibrium chemistry model used to predict the properties in a hydrogen - air flame are described below.

Four equilibrium reactions are assumed as follows:

$$H + H \underset{}{\overset{k_1'}{\rightleftharpoons}} H_2 \qquad \text{(A-1)}$$

$$O + O \underset{}{\overset{k_2'}{\rightleftharpoons}} O_2 \qquad \text{(A-2)}$$

$$H + OH \underset{}{\overset{k_3'}{\rightleftharpoons}} H_2O \qquad \text{(A-3)}$$

$$O + H \underset{}{\overset{k_4'}{\rightleftharpoons}} OH \qquad \text{(A-4)}$$

The six species involved in these reactions are considered to be present with nitrogen which is inert. In developing the equations to predict the equilibrium concentration of the species, two quantities are defined, namely:

$$F = m_{O_2} + m_O + \frac{W_O}{W_{H_2O}} m_{H_2O} + \frac{W_O}{W_{OH}} m_{OH} \qquad \text{(A-5)}$$

$$f = m_{H_2} + m_H + \frac{W_{H_2}}{W_{H_2O}} m_{H_2O} + \frac{W_H}{W_{OH}} m_{OH} \qquad \text{(A-6)}$$

where F is the total mass fraction of oxygen in any form and f is the total mass fraction of hydrogen in any form. Since the molecular weight of the various oxygen species is approximately equal to that of nitrogen, it is assumed that the coefficient of turbulent diffusion of the chemical species are equal to each other at every point in the flow. A well known consequence is that f is linearly related to m_{N_2} and the constants in the relation can be determined from the boundary conditions:

$$\frac{m_{N_2}}{m_{N_2,air}} + \frac{m_{O_2}}{m_{O_2,air}} = 1 - f \qquad \text{(A-7)}$$

The total mass fraction of all elemental species must be unity which gives,

$$F + m_{N_2} + f = 1 \qquad \text{(A-8)}$$

Also,

$$F = q\ (1 - f) \qquad \text{(A-9)}$$
$$\text{with } q = m_{O_2,air} = 0.232$$

Therefore, if f is known, F can be determined by equation (A-9).

From thermodynamic considerations the equilibrium constant K_p, for the reaction:

$aA + bB \underset{\leftarrow}{\overset{K_p}{\rightarrow}} cC$ is defined by,

$$K_p = \frac{x_C^c}{x_A^a\ x_B^b}\, p^{c-a-b} \qquad \text{(A-10)}$$

where x stands for concentration and the pressure p is in atmospheres. For each of the four reactions (A-1) to (A-4) in the present model c-a-b = -1. Expressing the concentrations in terms of mass fractions by noting that,

$$m_i = \frac{Wi}{W}\, x_i \qquad \text{(A-11)}$$

where W is the molecular weight of the mixture we get:

$$K_p' = K_p p^W \frac{W_C^c}{W_A^a\ W_B^b} = \frac{m_C^c}{m_A^a\ m_B^b} \qquad \text{(A-12)}$$

Thus the equilibrium equations for the reactions (A-1) to (A-4) can be written:

$$K_1' = \frac{m_{H_2}}{m_H^2} \qquad \text{(A-13)}$$

$$K_2' = \frac{m_{O_2}}{m_O^2} \qquad \text{(A-14)}$$

$$K_3' = \frac{m_{H_2O}}{m_H m_{OH}} \qquad \text{(A-15)}$$

$$K_4' = \frac{m_{OH}}{m_O m_H} \qquad \text{(A-16)}$$

The condition of equilibrium is expressed using four equilibrium constants for the four chemical reactions. If thermodynamic equilibrium prevails, the K's take values which depend upon temperature alone. In the above set of equations there are seven unknowns (m_{H_2}, m_{O_2}, m_H, m_O, m_{OH}, m_{H_2O} and F; f being given) and seven equations (A-5, A-6, A-8, A-13, A-14, A-15, A-16). The problem is therefore soluble.

The remaining discussion defines the solution procedure.

Derivation of Solution Procedure

The present procedure is based on the reduction of the number of variables under consideration. Two equations are derived as follows:

Equations (A-13 - A-16) are solved to give the relationships:

$$m_H = \frac{1}{\sqrt{K_1'}} \sqrt{m_{H_2}} \qquad \text{(A-17)}$$

$$m_O = \frac{1}{\sqrt{K_2'}} \sqrt{m_{O_2}} \qquad \text{(A-18)}$$

$$m_{H_2O} = \frac{K_3' K_4'}{K_1' \sqrt{K_2'}} m_{H_2} \sqrt{m_{O_2}} \qquad \text{(A-19)}$$

$$m_{OH} = \frac{K_4'}{\sqrt{K_1' K_2'}} \sqrt{m_{H_2}} \sqrt{m_{O_2}} \qquad \text{(A-20)}$$

It is convenient to define the following parameters*:

$$\bar{A} = \frac{1}{\sqrt{K_1'}} \qquad \text{(A-21)}$$

$$\bar{B} = \frac{1}{\sqrt{K_2'}} \qquad \text{(A-22)}$$

$$\bar{C} = \frac{K_3' K_4'}{K_1' \sqrt{K_2'}} \qquad \text{(A-23)}$$

$$\bar{D} = \frac{K_4''}{\sqrt{K_1' K_2'}} \qquad \text{(A-24)}$$

---

*These depend upon temperature alone; therefore, they can be tabulated right at the start.

Using equations (A-17 to A-20) to eliminate m_O, m_{H_2O}, m_H and m_{OH} from equations (A-5) and (A-6) gives:

$$F = m_{O_2} + \sqrt{m_{O_2}} \left(\bar{B} + \frac{8}{9} \bar{C} m_{H_2} + \frac{16}{17} \bar{D} \sqrt{m_{H_2}}\right) \qquad \text{(A-25)}$$

$$f = m_{H_2} \left(1 + \frac{1}{9} \bar{C} \sqrt{m_{O_2}}\right) + \sqrt{m_{H_2}} \left(\bar{A} + \frac{1}{17} \bar{D} \sqrt{m_{O_2}}\right) \qquad \text{(A-26)}$$

Where the definitions given by equations (A-21 to A-24) have been used.

These equations have the form of a quadratic equation:

$$\bar{a}u^2 + \bar{b}u + \bar{c} = 0$$

with solution

$$u = \frac{-2\bar{c}}{\bar{b} \pm \sqrt{\bar{b}^2 - 4\bar{a}\bar{c}}} \qquad \text{(A-27)}$$

Note that $\bar{a}$ and $\bar{b}$ are always positive and $\bar{c}$ is always negative. Since $u > 0$, the physically meaningful root is the one with the positive sign. This particular form of quadratic expression is chosen since it does not require subtraction and gives greater precision. Using equation (A-27) to express the solution of equations (A-25) and (A-26) gives:

$$\sqrt{m_{O_2}} = \frac{F}{\left[\frac{\bar{B} + \frac{8}{9} \bar{C} m_{H_2} + \frac{16}{17} \bar{D} \sqrt{m_{H_2}}}{2}\right] + \sqrt{\left[\frac{\bar{B} + \frac{8}{9} \bar{C} m_{H_2} + \frac{16}{17} \bar{D} \sqrt{m_{H_2}}}{2}\right]^2 + F}} \qquad \text{(A-28)}$$

$$\sqrt{m_{H_2}} = \frac{f}{\left[\frac{\bar{A} + \frac{1}{17}\bar{D}\sqrt{m_{O_2}}}{2}\right] + \sqrt{\left[\frac{\bar{A} + \frac{1}{17}\bar{D}\sqrt{m_{O_2}}}{2}\right]^2 + (1 + \frac{1}{9}\bar{C}\sqrt{m_{O_2}})f}} \quad \text{(A-29)}$$

Equations (A-28) and (A-29) contain the unknowns m_{O_2} and m_{H_2}. Before detailing the solution procedure several properties of these equations will be discussed. Table A-1 gives the values of K_1', K_2', K_3', K_4', $\bar{A}$, $\bar{B}$, $\bar{C}$ and $\bar{D}$ for the temperatures from 100 to 6000K at a constant pW product of 2.5 (corresponding approximately to 1/10 atmosphere). Note that while the individual constants vary from less than 1 to 10^{100}, the groups appearing in equations (A-28) and (A-29) vary much less and can be easily processed on a digital computer. Second it is to be observed that the equations have been derived so that a 'physical' relationship has been established between m_{O_2} and F, and m_{H_2} and f, i.e. as $F \to 0$, $m_{O_2} \to 0$, and as $f \to 0$, $m_{H_2} \to 0$. It should also be observed that m_{O_2} and m_{H_2} can never be less than zero or greater than 1. Finally, neither equation becomes indefinite as m_{H_2} or m_{O_2} approach zero. Thus, the equations are well-behaved and can be readily solved for wide variations in temperature and pressure. The solution procedure is described next. A value of m_{H_2} is guessed in the following way. If the value at the equivalent upstream station is known, then that value is used; otherwise, a value of zero will always lead to a converged solution. This assumed value of m_{H_2} is substituted into equation (A-28) which yields m_{O_2}. Then the computed value of m_{O_2} is substituted into equation (A-29) which allows calculation of a new value of m_{H_2}. The assumed and calculated values of m_{H_2} are compared. If these values differ by more than a specified convergence criterion, the calculated value of m_{H_2} is taken as the assumed value and the process described above is repeated until convergence is obtained. The behaviour of this solution technique is shown in Figure A-1. This figure shows with the broken line a plot of m_{H_2}

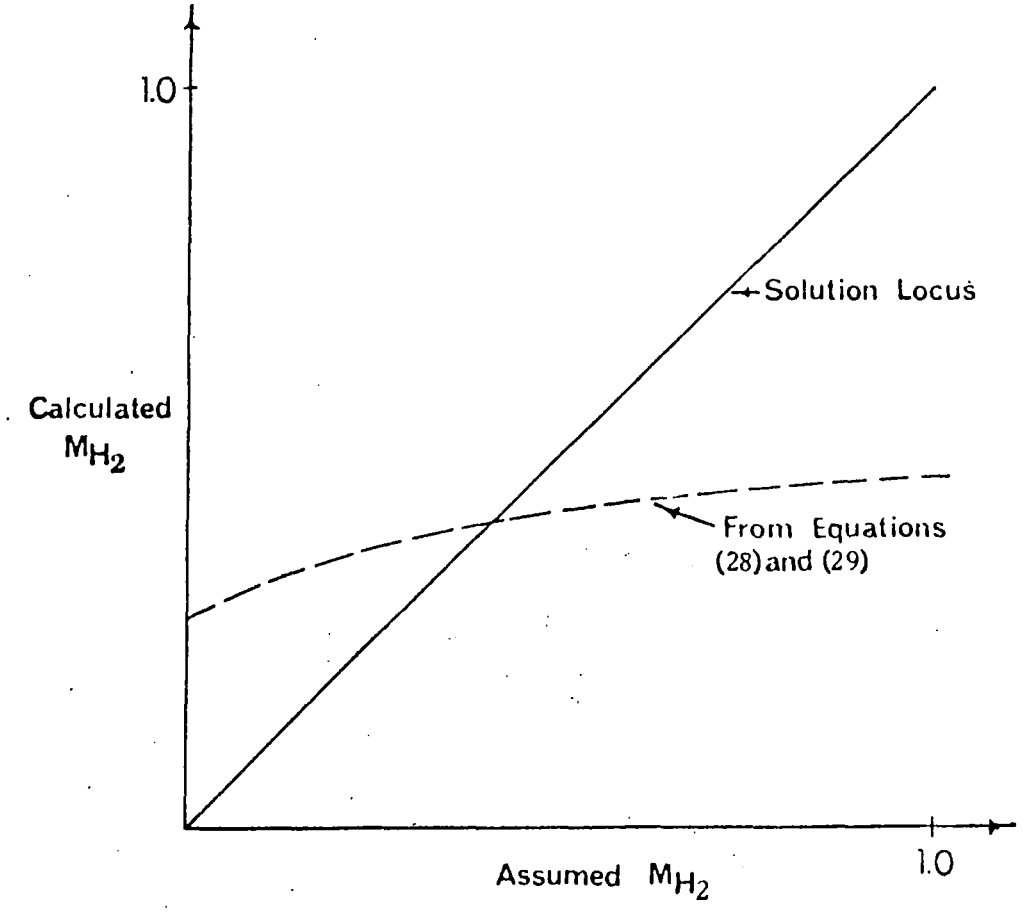


FIGURE A-1: GRAPHICAL PLOT OF TRIAL-AND-ERROR SOLUTION

calculated versus m_{H_2} assumed. The correct value is achieved when the two values are equal. The locus of points for this situation is a straight line with a slope of unity. If m_{H_2} assumed is less than the correct value, the figure shows that the calculated value will always be larger. Thus, when this calculated value of m_{H_2} is taken as the assumed value, the resulting newly calculated value will be closer to the correct one. The same argument can be made to show that if the initial assumed value of m_{H_2} is too large, the iteration process will again cause convergence to the correct one. Great precision can be obtained with this method. The convergence criterion for the calculation is:

$$|m_{H_2} \text{ calculated} - m_{H_2} \text{ assumed}| < 0.001\ m_{H_2} \text{ calculated}$$

Greater precision can be easily achieved by a stricter convergence criterion. However, the present one is sufficient for most practical calculations.

It may be concluded that the method offers a reliable, simple and extremely fast technique for solving the equilibrium equations arising from the chemical model considered in this work.

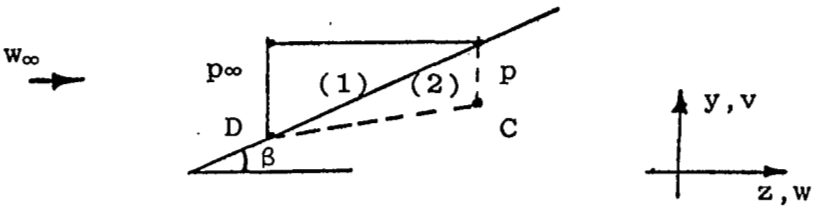
TABLE A-1. NUMERICAL VALUES OF EQUILIBRIUM CONSTANTS

Temp	K_1'	K_2'	K_3'	K_4'	$\bar{A}$	$\bar{B}$	$\bar{C}$	$\bar{D}$
200	5.0+100	3.1E+99	2.6+100	2.6+100	4.4E-51	1.7E-50	2.42E+50	1.95E+00
400	2.8E+52	2.7E+58	3.2E+51	6.2E+59	5.9E-27	6.0E-30	4.30E+29	2.19E+04
600	2.3E+33	4.3E+36	5.8E+32	9.0E+37	2.0E-17	4.7E-19	1.09E+19	8.46E+02
800	5.9E+23	4.9E+25	2.2E+23	9.3E+26	1.2E-12	1.4E-13	4.95E+13	1.56E+02
1000	9.7E+17	1.2E+19	4.5E+17	2.2E+20	1.0E-09	2.7E-10	2.94E+10	5.94E+01
1200	1.2E+14	5.0E+14	7.0E+13	8.2E+15	8.7E-08	4.4E-08	2.14E+08	3.14E+01
1400	2.1E+11	3.5E+11	1.2E+11	5.4E+12	2.1E-06	1.6E-06	5.22E+06	1.81E+01
1600	1.7E+09	1.1E+09	1.1E+09	2.2E+10	2.4E-05	2.5E-05	3.67E+05	1.32E+01
1800	3.9E+07	2.1E+07	2.7E+07	3.0E+08	1.5E-04	2.1E-04	4.53E+04	9.45E+00
2000	1.9E+06	7.0E+05	1.4E+06	9.8E+06	7.2E-04	1.1E-03	8.63E+03	7.76E+00
2200	1.5E+05	4.3E+04	1.2E+05	5.8E+05	2.5E-03	4.8E-03	2.24E+03	6.96E+00
2400	1.9E+04	4.2E+03	1.6E+04	5.5E+04	7.0E-03	1.5E-02	0.71E+03	5.77E+00
2600	3.4E+03	5.8E+02	2.8E+03	7.6E+03	1.7E-02	4.1E-02	2.60E+12	5.30E+00
2800	7.5E+02	1.0E+02	6.4E+02	1.3E+03	3.6E-02	9.6E-02	1.11E+02	4.49E+00
3000	2.0E+02	2.4E+01	1.74+02	3.1E+02	7.0E-02	2.0E-01	5.37E+01	4.34E+00
3200	6.3E+01	6.8E+00	5.7E+01	8.5E+01	1.2E-01	3.8E-01	2.95E+01	3.87E+00
3400	2.3E+01	2.1E+00	2.1E+01	2.7E+01	2.0E-01	6.7E-01	1.70E+01	3.62E+00
3600	9.3E+01	7.9E-01	8.6E+00	9.8E+00	3.2E-01	1.1E+00	1.02E+01	3.45E+00
3800	4.1E+00	3.2E-01	3.8E+00	3.9E+00	4.9E-01	1.7E+00	6.38E+00	3.25E+00
4000	1.9E+00	1.4E-01	1.8E+00	1.7E+00	7.0E-01	2.6E+00	4.30E+00	3.09E+00
4200	1.0E+00	6.8E-02	9.8E-01	8.3E-01	9.8E-01	3.8E+00	3.12E+00	3.09E+00
4400	5.5E-01	3.5E-02	5.4E-01	4.2E-01	1.3E+00	5.3E+00	2.20E+00	2.89E+00
4600	3.2E-01	1.8E-02	3.1E-01	2.2E-01	1.7E+00	7.2E+00	1.59E+00	2.69E+00
4800	1.9E-01	1.0E-02	1.9E-01	1.3E-01	2.2E+00	9.6E+00	1.30E+00	2.74E+00
5000	1.2E-01	6.4E-03	1.2E-01	7.7E-02	2.8E+00	1.2E+01	9.62E-01	2.59E+00
5200	7.9E-02	4.0E-03	7.8E-02	4.8E-02	3.5E+01	1.5E+01	7.49E-01	2.52E+00
5400	5.3E-02	2.5E-03	5.3E-02	3.1E-02	4.3E+00	1.9E+01	6.20E-01	2.53E+00
5600	3.6E-02	1.7E-03	3.6E-02	2.0E-02	5.2E+00	2.4E+01	4.85E-01	2.49E+00
5800	2.6E-02	1.1E-03	2.6E-02	1.4E-02	6.1E+00	2.9E+01	4.22E-01	2.47E+00
6000	1.8E-02	8.1E-04	1.8E-02	9.8E-03	7.2E+00	3.5E+01	3.44E-01	2.47E+00

APPENDIX B

Free-Stream Boundary Conditions in Supersonic Flows

(a) Consider the effect of a pressure wave of angle β on a stream of velocity w_∞ (supposing that $v_\infty = 0$ and $u_\infty = 0$).



The v-momentum equation for the domain ABCD (where AB and CD are stream surfaces) is:

$$w_\infty \rho_\infty (v_\infty - v) = (p_\infty - p) / \tan\beta \qquad \text{(B-1)}$$

$$\tan\beta = (w_2 - w_\infty)/(v_2 - v_\infty)$$

The wave angle can be related to the Mach number by:

$$\tan\beta = 1/\sqrt{M_\infty^2 - 1} \qquad \text{(B-2)}$$

so that:

$$v = \frac{p - p_\infty}{\rho_\infty w_\infty}\sqrt{M_\infty^2 - 1} \qquad \text{(B-3)}$$

(b) The energy equation for a perfect gas gives:

$$\frac{u_b^2}{2} + \frac{\gamma p_b}{(\gamma-1)\rho_b} = \frac{w_\infty^2}{2} + \frac{\gamma p_\infty}{(\gamma-1)\rho_\infty} \qquad \text{(B-4)}$$

where U_b denotes the resultant velocity at the boundary. For an isentropic flow,

$$\frac{p_b}{\rho_b^\gamma} = \frac{p_\infty}{\rho_\infty^\gamma} \quad , \text{(B-5)}$$

whence: $$\rho_b = \left(\frac{p_b}{p_\infty}\right)^{1/\gamma} \rho_\infty \quad , \text{(B-6)}$$

so that:

$$\frac{p_b}{\rho_b} = \frac{p_b}{(p_b/p_\infty)^{1/\gamma}\,\rho_\infty} = \left(\frac{p_b}{p_\infty}\right)^{(1 - 1/\gamma)} \frac{p_\infty}{\rho_\infty} \quad , \text{(B-7)}$$

Substitution of (B-7) into (B-4) gives:

$$u_b = \sqrt{w_\infty^2 + 2\,\frac{\gamma}{\gamma-1}\,\frac{p_\infty}{\rho_\infty}\left\{1 - \left(\frac{p_b}{p_\infty}\right)^{\frac{\gamma-1}{\gamma}}\right\}} \quad , \text{(B-8)}$$

and of course

$$w_b = \sqrt{u_b^2 - v_b^2 - u_b^2} \quad \text{(B-9)}$$

APPENDIX C

List of FORTRAN Variables

Notes

1. Star rating

   This list classifies variables as having general importance or being merely of local significance. The latter variety is marked with a dash (-). In the former variety, each variable is given a star rating of one (*), two (**) or three (***) stars. This indicates that the variable is appropriate to the problem-dependent (*), physical-modelling (**), or the main-machinery (***) part of the program.

2. Subscripted variables

   Subscripts to variables are shown only when necessary, in order to explain the meaning of the variable. In general therefore, the subscript status of each variable should be understood from the column headed NATURE.

3. Symbols

   Wherever possible, the symbols corresponding to FORTRAN variables, which are used in the text, are also listed.

NO	VARIABLE	NATURE	STAR RATING	SYMBOL	MEANING
1	A(I)	REAL,ARRAY	***		Transformed coefficient in TDMA operation
2	ADIN	REAL,	*		Dissipation rate at inlet
3	ADS(IJ)	REAL,ARRAY	***	ε	Dissipation rate
4	AGEOM	REAL,	*	-	Factor in grid expansion
5	AK	REAL,	**	K	Mixing-length constant
6	AKE(IJ)	REAL,ARRAY	***	k	Turbulence energy
7	AKFAC	REAL,	-		Factor relating k to mean motion energy
8	AKIN	REAL,	*		Inlet kinetic energy
9	ALX,ALXM, ALXP,ALY ALYM,ALYP, ALZ,ALZ1	REAL,	-	ξ L_e, L_s^{η} etc	Quantities representing the convective coefficients in the finite-difference equations
10	AMUREF	REAL,	*		Reference laminar viscosity
11	AMUT(IJ)	REAL,ARRAY	**	μ_t	Turbulent viscosity
12	ARAT	REAL,	*		Ratio of upstream to downstream areas
13	AREA	REAL,	-		Area of control-volume face
14	AXM,AXP, AYM,AYP, AZ	REAL,ARRAY	***	A_W, A_E, A_S, A_N, $L_{P,U}^{\zeta}$	Coefficient of finite-difference equations
15	B	REAL,ARRAY	***		Transformed coefficient in TDMA operation
16	BXE	REAL,	**	$\Delta\xi_E$	Width of integration plane in the ξ-direction
17	BXEU	REAL,	*		Upstream value of BXE
18	BYN	REAL,	**	$\Delta\eta_N$	Width of integration plane in the η-direction
19	BYNU	REAL,	*		Upstream value of BYN
20	CD	REAL,	**	C_D	Constant in turbulence model

NO	VARIABLE	NATURE	STAR RATING	SYMBOL	MEANING
21	CDQR,CDRT, CDTQ	REAL,	**	$C_D^{\frac{1}{4}}, C_D^{\frac{1}{2}}$ $C_D^{\frac{3}{4}}$	Roots of CD
22	CP	REAL,	*	C_p.	Specific heat
23	CPDCV	REAL	*	C_p/C_v	Specific heat at constant pressure divided by specific heat at constant volume
24	CX,CXP, CY,CYP, CZ,CZP	REAL, CY only as ARRAY	-		Temporary storage for finite-difference coefficients
25	C1,C2	REAL,	*		Constants in turbulence model
26	CFS etc	REAL,	*		Local shear stress at South wall
27	CFSAV,etc	REAL,	*		Local normalised shear stress at South wall
28	DBXEDZ, DBYNDZ	REAL,	**	$\frac{d}{dz}(\Delta\xi_E)$, $\frac{d}{dz}(\Delta\eta_N)$	Rates of growths of BXE, BYN with respect to dz
29	DEN	REAL,	**	ρ	Reference density of fluid
30	DHED	REAL,	*		Dynamic Head
31	DHEDIN	REAL,	*		Value of DHED at inlet
32	DPDZ	REAL,	***	$\frac{\partial p}{\partial z}$	Pressure-gradient in the ζ-direction
33	DPDZU	REAL,	*		Upstream value of DPDZ
34	DU,DV,DW	REAL,ARRAY	***	D^U, D^V, D^W	Pressure-difference coefficients for the U,V & W velocities
35	DXWDZ, DYSDZ	REAL	**		Slopes of W & S boundaries
36	DZ	REAL,	***	$\Delta\zeta$	Forward step-size

NO	VARIABLE	NATURE	STAR RATING	SYMBOL	MEANING
37	DZU	REAL,	*		Upstream value of DZ
38	EE	REAL,	*	E	Constant in the law-of-the-wall
39	ETA	REAL,ARRAY	***	η	Non-dimensional y coordinate
40	EX	REAL,	*		Factor by which forward step size is incremented
41	F	REAL,ARRAY	***	ϕ	Store for dependent-variable values
42	FLOWIN	REAL,	*		Rate of mass inflow into the calculation domain
43	FLOINJ FLOINT	REAL,ARRAY	*		Mass flow rate injected by a jet through the south and north wall respectively
44	FLUXE, FLUXW, FLUXN, FLUXS	REAL,ARRAY	*		Fluxes of dependent variables on E,W,N,S boundaries
45	FRA, FRAM	REAL,	-		Fraction of boundary-layer width used in calculating forward step size. FRAM is the maximum value of FRA
46	FXM,FXP, FYM,FYP	REAL,ARRAY	***		Interpolation factors to indicate distance of a pressure node from the neighbouring velocity locations
47	GAM	REAL,ARRAY	***	Γ_ϕ	Store for diffusion coefficients
48	GAMA	REAL,	-		Local value of GAM at locations where it is not stored
49	GAME, GAMW, GAMS, GAMN	REAL,ARRAY	*	$\Gamma_{\phi,wall}$	Boundary values of GAM to compute corresponding FLUX's

NO	VARIABLE	NATURE	STAR RATING	SYMBOL	MEANING
50	GASCON	REAL,	*	R	Universal gas constant
51	GREAT	REAL,	-		Large number, used to fix values to desired levels and in limiting overflows; 10^{30}
52	GX,GY GZ	REAL,ARRAY	**		Mass velocities in the ξ, η and ζ-directions
53	HO	REAL,ARRAY	*	h_i^o	Enthalpy of formation
54	I	INTEGER,	***		Index indicating position in the ξ-direction
55	ICJUMP	INTEGER,	*		Index, controlling calculation of wall fluxes for purposes of printout only
56	IINJ, IINJT	INTEGER,	*		Indices to control entry to INJMOD and INJMOT, respectively
57	IJ,IJE IJN,IJNW, IJS,IJSE, IJW				Computed subscripts to replace (I,J),(I+1,J) (I,J+1),(I-1,J+1),(I-1, J),(I+1,J-1),(I-1,J)
58	IJREF	INTEGER,	***		Location of grid node that is used as the reference for relative pressure
59	IJT	INTEGER,	**		Calculable subscript for T (=IJ+NFM(NVT))
60	IMAX	INTEGER,	***		Maximum value of I, for which storage locations are provided in the program
61	INJSTR, INJTOP	INTEGER,	*		Value of ISTEP at injection location,, for South and North wall, respectively
62	IPRINT (NV)	INTEGER,ARRAY	***		Values of a variable NV, printed only if the corresponding IPRINT is unity

NO	VARIABLE	NATURE	STAR RATING	SYMBOL	MEANING
63	ISOLVE (NV)	INTEGER,ARRAY	***		Index denoting whether the finite-difference equations of variable NV are solved (ISOLVE(NV) = 1) or not (ISOLVE(NV) = 0)
64	ISTEP	INTEGER,	***		Counter for forward steps
65	ISTR	INTEGER,	***		Value of I for the first internal storage location for a given variable
66	ISWP	INTEGER,	***		Index denoting the direction of sweep while performing the TDMA traverse in the ξ-direction
67	IXY	INTEGER,	***		Integer denoting whether the ξ-direction or the η-direction TDMA traverse is performed first
68	J	INTEGER,	***		Index denoting the position in the η-direction
69	JM(J)	INTEGER,ARRAY	***		(J-1)*IMAX ; used for subscript calculation
70	JMAX	INTEGER,	***		Maximum value of J, for which storage locations are provided
71	JSMAX	INTEGER,	*		J-location of SMAX
72	JSTR	INTEGER,	***		Value of J denoting the first internal location for a given variable
73	JSWP	INTEGER,	***		Index denoting the direction of sweep while performing the TDMA traverse in the η-direction

NO	VARIABLE	NATURE	STAR RATING	SYMBOL	MEANING
74	KBCE, KBCW, KBCN, KBCS	INTEGER,	***		Indices, denoting the nature of the E,W,N and S boundaries; = 1 for wall boundaries; = 2 for symmetry planes; = 3 for 'free' boundaries
75	L	INTEGER,	***		Number of grid lines minus one in the ξ-direction;
76	LASTEP	INTEGER,	*		The LAST STEP i.e. the maximum number that ISTEP can attain
77	LCV	INTEGER,	***		The number of main control volumes in the ξ-direction
78	LP1	INTEGER,	***		Number of grid points in the ξ-direction
80	M	INTEGER,	***		Number of grid lines minus one in the η-direction
81	MCV	INTEGER,	***		Number of control volumes in the η-direction
82	MP1	INTEGER,	***		Number of grid points in the η-direction
83	NFM(NV)	INTERGER,ARRAY	***		(NV-1)*IMAX*JMAX; used for subscript calculation
84	NFPMAX	INTEGER,	*		Maximum number of variables F, for which arrangement for Printout is available
85	NITERF	INTEGER,	**		Number of iterations on variables ϕ (i.e. F) other than velocities
86	NITERM	INTEGER,	**		Number of iterations on velocity components
87	NMU	INTEGER,	***		Index identifying GAM, the effective diffusion coefficient

NO	VARIABLE	NATURE	STAR RATING	SYMBOL	MEANING
88	NNV	INTEGER,	***		Number of variables for which storage in the F array is provided
89	NH	INTEGER,	***		Identifier of atomic hydrogen concentration
90	NH2	INTEGER,	***		Identifier of molecular hydrogen concentration
91	NH20	INTEGER,	***		Identifier of water vapor concentration
92	NN2	INTEGER,	***		Identifier of molecular nitrogen concentration
93	NO	INTEGER,	***		Identifier of atomic oxygen concentration
94	NOH	INTEGER,	***		Identifier of OH concentration
95	NO2	INTEGER,	***		Identifier of molecular oxygen concentration
96	NPJUMP	INTEGER,	*		Intervals of ISTEP after which a printout of main variables is obtained
97	NPP	INTEGER,	***		Index identifying p' in the F-array
98	NRHO	INTEGER,	***		Index identifying ρ (density)
99	NSWP (NV)	INTEGER, ARRAY	***		Number of pairs of TDMA sweeps for variable (NV)
100	NV	INTEGER,	***		Serial number of any variable ϕ stored in the F-array

NO	VARIABLE	NATURE	STAR RATING	SYMBOL	MEANING
101	NVF,NVD NVK,NVH	INTEGER,	***		Identifiers for hydrogen concentration,(in any form),dissipation rate ε, turbulence energy k, and enthalpy $\bar{h}$, in F
102	NVP,NVT, NVU,NVV, NVW	INTEGER	***		Identifiers for pressure p, temperature T, and velocity components u, v and w, respectively
103	P	REAL,ARRAY	***	p	Static pressure p
104	PI	REAL,	*	π	Constant
105	PIN	REAL,	*		Inlet value of p
106	PJAY	REAL,	*	P_ϕ	Resistance of laminar sublayer
107	PP	REAL,ARRAY	***	p'	Pressure correction
108	PR(NV)	REAL,ARRAY	***	$\sigma_{t,\phi}$	Effective Prandtl/ Schmidt number
109	PREF	REAL,	**		Pressure at reference grid node
110	PRLAM (NV)	REAL,ARRAY	***	σ_ϕ	Laminar Prandtl/Schmidt number
111	RELAX (NV)	REAL,ARRAY	***	f^ϕ	Relaxation factor for NV
112	RETRAN	REAL,	*		Transition Reynolds number
113	RHO(IJ)	REAL,ARRAY	***	ρ	Density
114	ROAR	REAL,	*		Density and control volume face area product
115	SMALL	REAL,	-		Small number used to trap the possibility of divisions by zero; 10^{-30} used

NO	VARIABLE	NATURE	STAR RATING	SYMBOL	MEANING
116	SP	REAL,ARRAY	***	S_P	One part of the linearised source term
117	STANS etc	REAL	*		Local Stanton numbers at South wall, etc.
118	STANSM etc	REAL	*		Mean Stanton number at South wall, etc
119	SU	REAL,ARRAY	***	S_U	A part of the linearised source term
120	TIN	REAL,	*		Inlet value of Temperature T
121	TITLE (NV)	REAL,ARRAY	***		Array storing 36-character alpha-numeric names of members of F
122	TINJ, TINJT	REAL	*		Inlet jet temperature at South and North walls respectively
123	TWAL	REAL,	*		Temperature of wall boundaries
124	TX,TY	REAL,	-	$T^{\xi};T^{\eta}$	Temporary store for the diffusive coefficients
125	U(IJ)	REAL,ARRAY	***	u	Velocity component in the ξ-direction
126	UIN	REAL,	*		Inlet value of u
127	V(IJ)	REAL,ARRAY	***	v	Velocity component in the η-direction
128	VIN	REAL,	*		Inlet value of v
129	VINJ, VINJT	REAL,	*		Velocity of jet injection at South and North walls, respectively
130	VOL	REAL,	-		Volume of control volume, surrounding a grid node

NO	VARIABLE	NATURE	STAR RATING	SYMBOL	MEANING
131	W(IJ)	REAL,ARRAY	***	w	Velocity components in the ζ-direction
132	WBAR	REAL,	*		Mean value of w across each plane of calculation
133	WIN	REAL,	*		Inlet value of w
134	WM	REAL,ARRAY	**		Molecular weight
135	ZD	REAL,	***		Downstream value of ζ at which calculations are currently being performed
136	ZLAST	REAL,	*		Last value of ζ at which calculations are to be performed
137	ZU	REAL,	***		Upstream value of ζ
138	ZETA	REAL,ARRAY	***	ξ	Non-dimensional x coordinate
139	ZINJ, ZINJT	REAL,	*		z-location of injection at South and North walls, respectively
140	ZRE	REAL,ARRAY	*		Values of z for which printout is desired

APPENDIX D

Listing of SHIP

The subroutines and their entry points are listed in the following order.

1. BLOCK
2. MAIN
3. ALLMOD
   - BEGIN
   - GAMOD
   - GEOMOD
   - UPSTRM
   - SOMOD
   - INJMOD
   - INJMOT
4. AUX
   - DENSTY
   - GAMMA
   - SOURCE
   - VISCOS
   - SPECIE
5. PRINT
6. SOLVE
7. STRIDA
   - STRIDO
   - STRID1
   - STRID2
8. STRIDB
   - STRID3
   - STRID4

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